NAME

ONIOM2PDB − Generates a PDB file from a Gaussian ONIOM file (input or output file)

SYNOPSIS

oniom2pdb [−**d?** (?:0˜3)] [−**e**] [−**ed** number] [−**g** *Gaussian_file_name*] [−**h**] [−**n** step_number] [−**o** *output_PDB_file_name*] [−**p** value] [−**pdb** *PDB_file_name*] [−**q**] [−**w**]

DESCRIPTION

This program generates a PDB file from a Gaussian input or log 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.
−**e**	When used, the partial charge of each atom in the ONIOM file will be appended to the end of each line in the output PDB file
−**ed** number	Defines the number of decimal places used for the partial charges in the output PDB file. Default is 2.
−**g** *Gaussian_file_name*	Gaussian file. Can be either an input file or log file.
−**h** −−**help**	Print full ONIOM2PDB documentation via perldoc. Cannot be used with other options.
−**n** step_number	Step number. When a given log file is from an optimization job, the user can choose which step along the optimization path is used to generate the new PDB file.
−**o** *output_PDB_file_name*	Output PDB file. Default name is *Gaussian_file_name*.pdb. For example, if *X.log* is Gaussian_file_name, the default output PDB file name is *X.log.pdb*.
−**p** value	Write value as the occupancy for each atom in the output PDB file. If this flag is not set, the occupancy from template PDB file (if there is any) will be kept.
−**pdb** *PDB_file_name*	Template PDB file. This file will be used as a template to generate the new PDB file with the coordinates from the given Gaussian job file.
−**q**	Run in quiet mode and do not print progress messages.
−**w**	If set, all the non-coordinate lines (not beginning with ATOM or HETATM) will be kept in the output pdb file. Otherwise, the ouput pdb file will contain coordinate lines only.

EXAMPLES

oniom2pdb

Called without any parameters, ONIOM2PDB will display usage information. If −**h** or −−**help** is passed, then the full ONIOM2PDB documentation is displayed via perldoc.

oniom2pdb −w −g foo.gjf −pdb T.pdb −o foo.pdb

ONIOM2PDB reads foo.gjf, then creates a PDB file named foo.pdb using T.pdb as a template. The −w flag tells ONIOM2PDB to keep all non-coordinate lines from the template PDB when writing the new PDB file.

oniom2pdb −w −g foo.gjf −pdb T.pdb −o foo.pdb −e −ed 3

ONIOM2PDB reads foo.gjf, then creates a PDB file named foo.pdb using T.pdb as template. The −w flag tells ONIOM2PDB to keep all non-coordinate lines from the template PDB when writing the new PDB file. Flag −e tells ONIOM2PDB to write out the partial charge in the B factor position. Each partial charge has three decimal places (−ed 3). Since the −p flag is not used, occupancy values from the template PDB will be kept. If occupancy values are not available from the template PDB, a value of 1.00 will be used.

NOTES
    ONIOM2PDB

VERSION
    1.2

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