NAME

PDB2ONIOM − Generates a Gaussian ONIOM input file from a PDB file

SYNOPSIS

pdb2oniom [**−d?** (?:0˜3)] [**−h**] [**−i** *filename*] [**−near** number] [**−o** *filename*] [**−q**] [**−resid** *listfile*]

DESCRIPTION

This program generates Gaussian ONIOM input files from PDB files. The program will obtain partial charges from the AMBER force field for the atoms in each residue.

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 PDB2ONIOM documentation via perldoc. Cannot be used with other options.

−i *filename*   PDB file to be used to generate the Gaussian ONIOM input file.

−near number   number is in Angstroms. Any residue with at least one atom within this distance of any atom in the core residues will be free to move during the optimization process (with flag 0 in the Gaussian ONIOM job file). Default is 6.0 A.

−o *filename*   New Gaussian ONIOM input file. The default is newGaussianfile.gjf.

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

−resid *listfile*   File containing the list of core residues. The distance between atoms and these core residues will be used to set up the optimization flags. The format of file 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

pdb2oniom

 Called without any parameters, PDB2ONIOM will display usage information. If **−h** or **−−help** is passed, then the full PDB2ONIOM documentation is displayed via perldoc.

pdb2oniom −i foo.pdb −o foo.gjf

 PDB2ONIOM reads foo.pdb, then creates a Gaussian ONIOM input file named foo.gjf. Since no core residue list file was provided, all atoms in foo.gjf are free to move during geometry optimization.

pdb2oniom −resid residfile −near 6.5 foo.pdb −o foo.gjf

 PDB2ONIOM reads foo.pdb, then creates a Gaussian ONIOM input file named foo.gjf. All atoms in any non-core residue within 6.5 angstrom of any core residue listed in residfile are are free to move during geometry optimization run by foo.gjf.

NOTES

PDB2ONIOM also generates a .onb file. This file contains the Gaussian ONIOM job setup and residue information. Do not delete this file. This file will be needed for programs SETMVFLG and TRANSGEOM.

SEE ALSO

SETMVFLG TRANSGEOM

VERSION

1.2

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