NAME

SETMVFLG − Resets the Gaussian optimization flags in a Gaussian ONIOM input file

SYNOPSIS

setmvflg [−**b**] [−**d?** (?:1˜3)] [−**h**] [−**i** *ONIOM_input_file*] [−**near** number] [−**o** *ONIOM_input_file*] [−**onb** *ONB_file_name*] [−**q**] [−**resid** *listfile*]

DESCRIPTION

This program resets the optimization flags (0 or −1) in a Gaussian ONIOM input file based on the ONB file (generated by pdb2oniom), core residues list file (listfile), and a distance from the core residues to define the moving region.

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.

−**b**	When set, the coordinates from the ONB file (generated from the original PDB file) will be used for setting the optimization flags. when not set (default), the coordinates from the Gaussian ONIOM input file will be used for setting the optimization flags.
	In either case, the generated Gaussian ONIOM input file has the same coordinates as the given Gaussian ONIOM input file.
−**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 SETMVFLG documentation via perldoc. Cannot be used with other options.
−**i** *ONIOM_input_file*	Gaussian ONIOM job file used for resetting the optimization flags.
−**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** *ONIOM_input_file*	Gaussian ONIOM input file with new optimization flag setup. Default is ONIOM_NEW_Moving_Flag.gjf.
−**onb** *ONB_file_name*	ONB file for SETMVFLG containing the residue information.
−**q**	Run in quiet mode and do not print progress messages.
−**resid** *listfile*	File that has the list of core residues. The distance between 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

setmvflg

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

setmvflg −i foo.gjf −onb foo.onb −resid corelist.txt −near 7 −o foonew.gjf

> SETMVFLG reads foo.gjf, foo.onb and corelist.txt files, and collects coordinates from foo.gjf, residue information from foo.onb file, and core residues information from corelist.txt. Then, SETMVFLG resets optimization flag so that all the residues within 7.0 Angstroms from any core residue are free to move during the geometry optimization, and creates a Gaussian input file named foonew.gjf with the new flag setup.

VERSION
1.0

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