

NAME

essebdb - ESSEB database management

VERSION

Version 0.1

Molecule Library Version 0.1

SYNOPSIS

essebdb input_pdb [-d *database_file*] [-h] [-m] [-n *notice_level*] [-o *header*]

DESCRIPTION

The ESSEB database stores protein conformations as a set of quaternions and translations that describe the angular orientation of each Secondary Structure Element (SSE) along with the position of the axis center. The quaternions and translation describe how to generate the conformation from an input pdb file, and therefore the same input file that is used to generate the database should be used as input to this program. In order to generate absolute positions, the original input file for ESSEB should have each SSE center placed at the ORIGIN with the SSE axis parallel to the Z-axis. This can be accomplished with the ESSEB option '-q'. The output files have any atoms that do not belong to an SSE (as specified by HELIX records) deleted. The PDB secondary structure, CONECT, and DSTRST records are maintained from the input file.

Currently, database management is limited to a dump of every database conformation to disk as a PDB file. For the format of the output filenames, see the -o parameter description. Databases written in vector format cannot be read.

PARAMETERS

-d *database_file*

Specify the name of the ESSEB database file. The default is "esseb.db"

-h Print out the man page for help

-m Do not merge continuous SSEs into a single axis. By default an SSE is merged with a second SSE if the terminal residue of one is the starting residue of another, or if the terminal residue of one comes just before the starting residue of another in terms of residue sequence numbers. *Note: if this option is set, the ending residue for one SSE may NOT be the starting residue for another.*

-n *notice_level*

Set the degree of program output. Use:

-n 0 No output
-n 10 Normal program output
-n 20 Parameters useful for reproducing the results
-n 30 All output

-o *header*

Specify the *header* for the output pdb files. The default is "esseb" The output files are named as *header.record_number.pdb*

FILE FORMAT

THE ESSEB database record format is:

$$w_1 \ i_1 \ j_1 \ k_1 \ x_1 \ y_1 \ z_1 \ \dots \ w_n \ i_n \ j_n \ k_n \ x_n \ y_n \ z_n$$

for input SSEs indexed 1-**n**. w is the real component of the quaternion, i , j , and k are the imaginary parts, and x , y , and z describe the SSE translation. These values are relative to conformations of the original input file. The output files are in PDB 2.2 format.

SEE ALSO

esseb(1)

AUTHORS

ESSEB was developed by W. Michael Brown and Jean-Loup Faulon