mkdssp

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NAME

mkdssp - Assign secondary structure to proteins

SYNOPSIS

mkdssp [OPTION] input [output]

DESCRIPTION

The DSSP program was designed by Wolfgang Kabsch and Chris Sander to standardize secondary structure assignment. DSSP is a database of secondary structure assignments (and much more) for all protein entries in the Protein Data Bank (PDB). mkdssp is the program that calculates DSSP entries from PDB entries. mkdssp does **not** predict secondary structure.

The original DSSP program wrote output in a fixed format, this version by default writes annotated mmCIF files, storing the secondary structure information in the _struct_conf category.

Since version 4.0 the mkdssp program also assigns PPII helices.

OPTIONS

The input file can be either mmCIF or PDB format and the file may be gzip compressed. Note that input files must be formatted correctly. E.g. PDB files must have a CRYST1 record. More info: https://www.wwpdb.org/documentation/file-format-content/format33/sect8.html#CRYST1

The output is optional, if omitted the output is written to *stdout*. If the name of the output file ends with either *.gz* or *.bz2* the output is compressed accordingly.

--output-format=[dssp|mmcif]

> If an output file is specified, the extension of the filename is used to choose to output format, but if it is unclear, mmcif is the default. Use this option to force output in either the old fixed column DSSP format or the new annotated mmCIF format.

--no-dssp-categories

> When writing mmCIF files, suppress the output of all dssp_ categories.

--min-pp-stretch

> This option can be used to define the minimal number of residues with PHI/PSI angles within the range required to assing a PP helix.

--write-other

By default the new format does not write the structure information for OTHER. Use this flag to change that.

--components

The knowledge of compounds is loaded from the CCD file *components.cif* that should have been installed by *libcifpp*. You can override that file by using this option.

--extra-compounds

As an addition to the standard *components.cif* file, you can add more files using this option. Files should be either in CCD format or should be CCP4 restraints files.

--mmcif-dictionary

The default mmCIF dictionary file is installed by the *libcifpp* library but you can override it using this option.

DETAILS

The DSSP algorithm assings secondary structure based on the energy calculated for H-bonds.

Table 1. Secondary Structures recognized

DSSP Code	mmCIF Code	Description
H	HELX_RH_AL_P	Alphahelix
B	STRN	Betabridge
E	STRN	Strand
G	HELX_RH_3T_P	Helix_3
I	HELX_RH_PI_P	Helix_5
P	HELX_LH_PP_P	Helix_PPII
T	TURN_TY1_P	Turn
S	BEND	Bend
' ' (space)	OTHER	Loop

BUGS

The mmCIF format currently lacks a lot of information that was available in the old format like information about the bridge pairs or the span of the various helices recognized. Also the accessibility information is left out.

If you think this information should be part of the output, please contact the author.

AUTHOR

Written by Maarten L. Hekkelman <maarten@hekkelman.com>

REPORTING BUGS

Report bugs at https://github.com/PDB-REDO/dssp/issues