

## NAME

**essebdrs** - ESSEB PDB distance restraints management

## VERSION

Version 0.1

Molecule Library Version 0.1

## SYNOPSIS

**essebdrs** input\_pdb [-a] [-c [*tolerance*]] [-d *drs\_file*] [-e *error\_adjust*] [-h] [-i] [-m] [-n *notice\_level*] [-o *output\_pdb*] [-r *res\_num*] [-s *serial1 serial2 [mindist] [maxdist]*] [-t *res\_num\_atom*] [-v] [-w *drs\_file*]

Parameters with optional arguments should be placed after mandatory commandline arguments.

## DESCRIPTION

ESSEB distance restraint I/O is handled via the addition of a DSTRST record to the PDB 2.2 file format (see FILE FORMAT). This program manages distance restraints within PDB files with options for adding and removing restraints. If the program is run with no parameters, the number of distance restraints in the file is output.

## PARAMETERS

**-a** Remove all distance restraints

**-c** [*tolerance*]

Check to see if the distance restraints in the input file are satisfied. Any violations are output. A signed *tolerance* for the *mindist* and *maxdist* error values can be specified.

**-d** *drs\_file*

Add distance constraints from a file formatted in the old restraint format. See FILE FORMATS for a description.

**-e** *error\_adjust*

Adjust the minimum and maximum error for every distance restraint by *error\_adjust*. Negative numbers are allowed

**-h** Print out the man page for help

**-i** Delete any atoms that do not belong to an SSE. This is useful for RMS fitting ESSEB conformations with a known structure. This does not need to be done for the input\_file to ESSEB because a similar function performed internally.

**-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** *output\_pdb*

Specify the filename for output of the modified PDB file. The default is to overwrite the input file.

**-r** *res\_num*

Add *res\_num* random distance restraints. Generated restraints will not be duplicates and will not exist between atoms in the same SSE. The minimum and maximum distance are set to the distance between the atoms in the *input\_pdb* file. NOTE: Currently, no method for seeding the random seed is available which can result in the same random numbers being generated consistently on some implementations.

**-s** *serial1 serial2 [mindist] [maxdist]*

Add a distance restraint between atoms with specified serial numbers. If no distance is specified, the *mindist* and *maxdist* are taken as the distance between the atoms in the input file. If *maxdist* is not specified, it is set equal to *mindist*. Adding a distance restraint that is already present between two atoms has NO effect, even if the distances are changed

**-t** *res\_num\_atom*

Add *res\_num\_atom* random distance restraints for each atom in the *input\_pdb* file. Generated restraints will not be duplicates and will not exist between atoms in the same SSE. The minimum and maximum distance are set to the distance between the atoms in the *input\_pdb* file. NOTE: Currently, no method for seeding the random seed is available which can result in the same random numbers being generated consistently on some implementations.

**-v** Generate CONECT records between atoms involved in distance restraints. This is useful for visualization.

**-w** *drs\_file*

Write out distance constraints in *input\_pdb* in the old format to the file *drs\_file*

## FILE FORMAT

THE DSTRST record format is:

```
DSTRST 1585 2315 23.24 27.24
```

Columns 1 - 6 "DSTRST"  
Columns 7 -11 Serial number of first atom  
Columns 12-16 Serial number of second atom  
Columns 17-26 Minimum distance between atoms (*Variable Precision*)  
Columns 27-36 Maximum distance between atoms (*Variable Precision*)

Functionality is also provided for reading in distance restraints in the old format which is space delimited:

```
DIST A134 CA A245 CA 14.32 18.32
```

Field 1 "DIST"  
Field 2 Chain ID and Sequence Number of first atom  
Field 3 Atom Name of first atom  
Field 4 Chain ID and Sequence Number of second atom  
Field 5 Atom Name of second atom  
Field 6 Minimum distance  
Field 7 Maximum distance

## EXAMPLES

**essebdrs** in.pdb

Get the number of distance restraints in *in.pdb*

**essebdrs** in.pdb **-d** constraints.dis

Add restraints specified in the old format from file *constraints.dis* to the file *in.pdb*

**essebdrs** in.pdb **-d** constraints.dis **-o** new.pdb

Same as above, except that *in.pdb* is unmodified and the file *new.pdb* is created to reflect the changes

**essebdrs** in.pdb

Remove all distance restraints from *in.pdb*

**essebdrs** in.pdb **-s** 52 105 10.3 14.3

Add a single distance restraint between atoms with serial numbers 52 and 105 such that the minimum distance between the atoms is 10.3 and the maximum distance is 14.3

**essebdrs** in.pdb **-t** 1

Add one random distance restraint per atom from *in.pdb*

**essebdrs** in.pdb **-i**

Delete any atoms from *in.pdb* that do not belong to an SSE

## SEE ALSO

esseb(1)

## AUTHORS

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