

# SHEBA Manual

## SHEBA (Structural Homology by Environment-Based Alignment)

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### Manual

This manual is for SHEBA version 3.11 only. The SHEBA 4.0 manual is not available yet.

SHEBA has the following options and the Help manual can be displayed by typing sheba in the command line. The sequence of the arguments does not affect the output. To learn how to use them, please click on each option and the example page will be displayed. Input and Output files are:

SHEBA(Version 3.0)

(Structural Homology by Environment Based Alignment)

sheba [.env or .pdb][.env or .pdb] : default

sheba -r [.env or .pdb] [.env or .pdb] : formatted row output

sheba -c [.env or .pdb] [.env or .pdb] : formatted column output

sheba -g [.env or .pdb] [.env or .pdb] : simple column output

sheba -x [.env or .pdb] [.env or .pdb] : transformation matrix output

sheba -p [.env or .pdb] [.env or .pdb] : permuted alignment

sheba -i [1-10][.env or .pdb] [.env or .pdb] : number of iterations

sheba -e [.pdb] : convert [.pdb] to [.env] file

sheba -t [.trf] [.env or .pdb] : transform [.env or .pdb] according to [.trf]

sheba -D [.list] : create [.db] file from [.list]

sheba -I [.db] : make one to many alignments with insertion

sheba -J [.db] : make one to many alignments without insertion

sheba -A [.env or .pdb] [.db] : one vs. [.db] alignments

sheba -L [.env or .pdb] [.list] : one vs. [.list] alignments

[.pdb] pdb file

[.env] environment file

[.db] database binary file

[.list] list of [.env] file names

[.trf] transformation matrix

J. Jung & B. Lee, Protein Eng. Vol. 13 pp.535-543, 2000.

**1. (.pdb): a flat PDB (ascii) format file.** If the PDB file name ends with (.ent), please rename it as (.pdb) so that SHEBA can recognize. If the PDB file comes from an NMR experiment, there might be more than one model and SHEBA only processes the first one.

**2. (.env): a PDB-like format with only alpha carbon coordinates and environment values.** Here is the example:

```
ATOM      0  CA  GLY  B  14      19.975   1.831  -7.534   0 89 99   0  -1
ATOM      1  CA  GLU  B  15      18.482  -1.197  -5.736   0 52 90   0  -1
ATOM      2  CA  ARG  B  16      17.295  -3.253  -8.746   0 89 98   0  -1
ATOM      3  CA  ARG  B  17      16.760  -6.143  -6.270   0 92 97   0  -1
ATOM      4  CA  ARG  B  18      14.019  -4.023  -4.631   0 37 82   0  -1
ATOM      5  CA  SER  B  19      12.084  -3.923  -7.929   0 61 89   0  -1
*****
```

Field Name: Definition

1. ATOM: Record type
2. atom id: The unique serial number of each atom.
3. atom name: IUPAC format; only alpha carbon is included.
4. residue name: IUPAC format.
5. chain: The chain to which the atom belongs.
6. residue id: The unique sequence number of each residue.
7. X coordinate: Orthogonal coordinates for X in angstroms.
8. Y coordinate: Orthogonal coordinates for Y in angstroms.
9. Z coordinate: Orthogonal coordinates for Z in angstroms.
10. secondary structure: 0: Coil 1: Helix 2: Sheet.
11. accessibility: Fraction of the solvent accessibility of the residue times 100.
12. polarity: Fraction of the environment polarity of the residue times 100.

**3. (.db): a concatenated and compressed form of a set of (.env) files.** This is a binary file.

**4. (.list): an ascii file that contains a list of structures to be compared.** Each line is one (\*.env) file name. Currently the default maximum number of files (NP) is set to 10000.

**5. (.trf): a file that contains a transformation matrix.** This is an ascii file. One can obtain this transformation matrix by giving a SHEBA command with "-x" option. This matrix transforms the second pdb coordinates toward the first.