

WEININGER WORKS™ SOFTWARE RELEASE NOTES

August 31, 2018

chainidPDB (version 1.1.0, previously named “change_chainid”)

- Added the ability to specify in finer detail which PDB components have their chain identifiers modified. Option '--model=' ('-a') was added to restrict modification to individual MODELS. Option '--from=' ('-f') now accepts either a simple list of chain identifiers or a triplet list of existing chain identifier, residue #, atom #. This triplet list allows flexible target specifications to be made that are either very restrictive (e.g., either a specific atom in a specific residue in a specific chain in a specific model) or more general (e.g., all records with residue 'N' regardless of chain identifier, etc.)
- Residue numbers for output chains are now automatically changed to be unique; new option '--noresiduechange' ('-x') may be used to prevent residue numbers from being changed.
- Output records are now automatically fixed to new chain order; new option '--nopositionchange' ('-p') may be used to prevent record position from being changed.
- New option '--map=' ('-m') may be used to generate a text file listing atom changes. "REMARK 250" lines are now added to the output PDB header specifying execution details.
- The character tilde (~) may be used as a short-hand for your home directory for all specified files.

combinePDB (version 1.1.1, previously named “combine”)

- Fixed the output of some error lines from stdout to stderr.
- Fixed the fourth connected atom index for output CONECT records.
- Residue numbers for output chains are now automatically changed to be unique; new option '--noresiduechange' ('-x') may be used to prevent residue numbers from being changed.
- Output records are now automatically fixed to new chain order; new option '--nopositionchange' ('-p') may be used to prevent record position from being changed.
- The character tilde (~) may be used as a short-hand for your home directory for all specified files.

deviation (version 1.0.1)

- The character tilde (~) may be used as a short-hand for your home directory for all specified files.

dist (version 1.0.2)

- The character tilde (~) may be used as a short-hand for your home directory for all specified files.

stripPDB (version 1.0.2)

- Added the program **stripPDB** to ww_freeware_bundle_3. **stripPDB** removes specified atoms from an input PDB file and writes a new output PDB file. The atoms to be removed may be specified with simple preset options, a simple list of chain identifiers, or a triplet list (as defined above for 'change_chainid').

twvistPDB (version 1.3.0, previously named “twvist”)

- Fixes made for more accurate positioning.
- Fixes made for more efficient execution.
- "REMARK 250" lines are now added to the output PDB header specifying execution details.
- The character tilde (~) may be used as a short-hand for your home directory for all specified files.

wwavePDB (version 1.0.4, previously named “wwaves”)

- **wwavePDB** is now freeware and is packaged with ww_freeware_bundle_3.
- Fixes made for more efficient execution.
- Added the ability to restrict set reference atoms by atom type with the command line option/value pairs: "--restrict=only_ref_atom" ('-r g'), "--restrict=only_ref_hetatm" ('-r h'), and "--restrict=ref_any_type" ('-r i').
- The character tilde (~) may be used as a short-hand for your home directory for all specified files.