

# MCCE Output Files

As part of the standard four steps, MCCE produces a number of files associated with the initial protein output. These are best understood to be members of six categories:

**Input:** The given PDB file. Often, MCCE programs will symbolically link the name "prot.pdb" to the input PDB file.

**Output:** Results of MCCE computation, to be interpreted by the user.

**Records:** Preserved information about the run.

**Instructions:** Files that control how MCCE runs. run.prm

**Control:** "Midpoint" files to preserve information between steps.

**Progress:** Benchmark files to keep track of what processes are occurring, and whether the run is succeeding.

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## Step-by-Step Output

### Program start and Initialization

Input files:

- run.prm: mcce control file
- param: parameter directory (specified in run.prm)
- extra.tpl: extra parameters. Often used to correct for bias. (optional, specified in run.prm)
- new.tpl: temporary parameter file for unrecognized cofactors. (optional, created by step 1 if unknown residues are present)

### Step 1: Formatting PDB File

Input files:

- PDB file
- name.txt
- list\_rot.gold (still?)

Output files:

- `acc.res`: solvent accessibility of residues
- `acc.atm`: solvent accessibility of atoms
- `new.tpl`: parameter file template of unrecognized cofactors (not always created)
- `head1.lst`: summary of rotamer making policy of residues (optionally used by step 2? how does that work?)
- `step1_out.pdb` (used by step 2):

## Step 2: Making Rotamers

Input files:

- `step1_out.pdb`: input structure of step 2 in mcce extended PDB format
- `head1.lst`: rotamer making policy of residues

Output files:

- `progress.log`: progress report file. Dynamically updated
- `rot_stat`: rotamer making statistics, dynamically updated
- `head2.lst`: summary of rotamers made in step 2 (optionally used by step 3)
- `step2_out.pdb`: step 2 output file with multiple rotamers in extended PDB format

## Step 3: Calculate the Energy Lookup Table

Input files:

- `step2_out.pdb`: Input instructions of step 3 in MCCE extended PDB format

Output files:

Alphabetized list

**acc.atm/acc.res** (Control/Output) - Gives the percent surface accessibility to the solvent of the atom/residue. Used to make rotamers.

**energies (Control)** - Self and pairwise energies generated during step 3.

**entropy.out** -

**err.log (Progress)** - Similar to `progress.log`, terminal output is moved here in the event of an error. Usually empty.

**fort.38 (Output)** - The name is a reminder that MCCE's origins were in Fortran.

**head1.lst/head2.lst/head3.lst (Control)** - `head1.lst` is created by step 1, and can be modified to reduce the number of conformers made in step 2. `head2.lst` is a summary of rotamers made in step

2.

**mc\_out (Progress)** - Provides details about the Monte Carlo process.

name.txt (Instructions) - The file referenced by mcce when renaming atom names, residue names, sequence number, and chain ID.

**param** - How

**pK.out (Output)** - Sampling across different pHs

**prot.pdb (Input)** - The name MCCE often uses in reference to the original input file.

**respair.lst** - Records the pairwise energy for each pair of conformers.

**rot\_stat (Progress)** - Provides statistics about rotamer creation.

**run.log (Record)** - Keeps a record of terminal output from steps.

**run.prm (Instructions)** - Created by step 1 if not provided- grants extra control over MCCE settings. For example, by default, the pH titration occurs along whole numbers from 0 - 14. The TITR settings can be edited to reduce the range of the pH titration, increase the points of titration, and more.

**run.prm.record** - Records the full run.prm details for each step. **CAUTION: If different settings are used on different runs in the same direct, run.prm.record may not capture the changes to the settings.**

**step0\_out.pdb/step1\_out.pdb/step2\_out.pdb** - Restructured versions of the input file. step0\_out deletes any header information (e.g., the headers included in RCSB downloads of PDB files). step1\_out renames residues according to a file called name.txt, including the opening and concluding residues of a sequence to NTR and CTR, respectively. step2\_out.pdb expands the list to include alternative conformers as well.

**sum\_crg.out** - Records information about the net charge of the PDB's residues at each pH titration.

**vdw0.lst** -

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