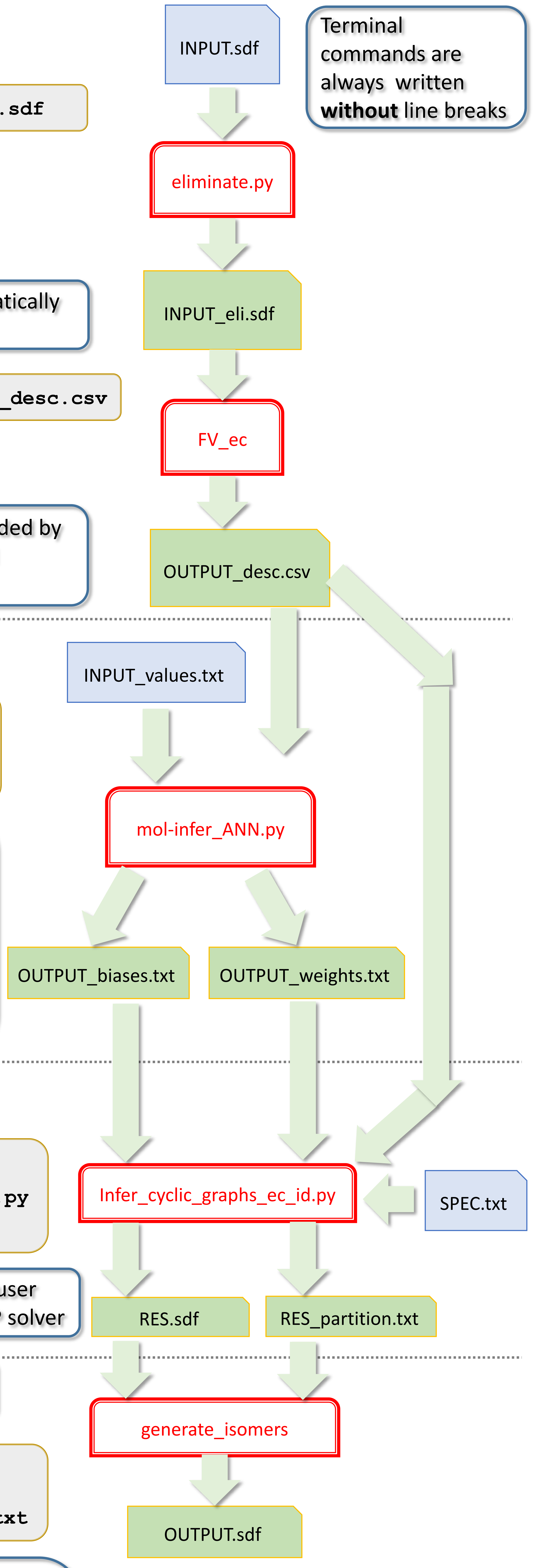
Files and Flow of Data in the Model for Inferring Cyclic Chemical Graphs

Used symbols and conventions

- 🟦 Files provided by the User
- 🟩 Files produced by the programs
- 🟥 Executable program
- `Terminal command`



Terminal commands are always written **without** line breaks

Module 1 (Calculating Feature Vectors)

```
python eliminate.py INPUT.sdf
```

The extension "_eli.sdf" is automatically added to the input file name.

```
./FV_ec INPUT_eli.sdf OUTPUT_desc.csv
```

The name of the output file is decided by the user and part of the command arguments.

Module 2 (Training an ANN)

```
python mol-infer_ANN.py
  INPUT_FV.csv
  INPUT_values.csv
  OUTPUT 20 10
```

- The suffixes "_biases.txt" and "_weights.txt" are added automatically.
- The filename "OUTPUT" is decided by the user.
- The constructed ANN has 2 hidden layers with 20 and 10 nodes each.

Module 3 (MILP)

```
python
  infer_cyclic_graphs_ec_id.py
  OUTPUT 42 SPEC.txt RES 1
```

-"42" is a target value given by the user
- "1" is a selection of CPLEX as MILP solver

Module 4 (Generating Graph Structures)

```
./generate_isomers
  RES.sdf 10 100000 5 100
  OUTPUT.sdf RES_partition.txt
```

-"10" specifies 10 seconds as a computation time limit for each stage
- "100000" is an upper bound on feature vectors stored in memory
- "5" is the number of sample graphs stored for each feature vector
- "100" is an upper bound on the number of resulting graphs

"OUTPUT.sdf" is the final result of this model.
In this example, it has up to 100 cyclic chemical graphs that are chemically isomorphic to the graph given in the file "RES.txt", and have target value "42".