To run examples:

1. Run all examples in this directory.

a. “python runAllExamples.py”

b. output files from input files in inSmi/ will be \*\_fromSmiles.cif and

\*\_fromSmiles.pdb

c. output files from input files in inMol/ will be \*\_ fromMol.cif and

\*\_fromMol.pdb.

d. output files from input files in inMmcif/ will be \*\_ fromMmcif.cif

and \*\_ fromMmcif.pdb

2. Run an individual example input file.

a. Run an input file from a SMILES file at inSmi/.

i. E.g. “acedrg –i inSmi/DB00201.smiles –o DB00201

ii. The output files are DB00201.cif (the dictionary file) and DB00201.pdb (the coordinate file)

b. Run an input file from a Mol file at inMol/.

i. E.g. “acedrg –m inMol/DB00201.mol –o DB00201

ii. The output files are DB00201.cif (the dictionary file) and DB00201.pdb (the coordinate file)

c. Run an input file from a mmcif file at inMmcif/

i. E.g. “acedrg –c inMmcif/DB00201.cif –o DB00201

ii. The output files are DB00201.cif (the dictionary file) and DB00201.pdb (the coordinate file)