This software provides code to accompany:

Covariance in protein multiple sequence alignments using groups of columns as the fundamental unit for computation - (submitted)

You will need

(1) a recent version of Java (at least 1.6) (http://www.oracle.com/technetwork/java/index.html)

 (2) The McBasc algorithm and COBS algorithm has a requirement for the file Maxhom_McLachlan.metric. This file should be in the subdirectory "data" where you unzipped the distribution zip file.

(3) There is a file in the src directory of the distribution called Energetics.properties. This file needs to be in a directory in your classpath and needs to be edited so that it points to the correct place on your hard drive

You'll need to edit the Energetics.properties file so that the following lines are defined:

```
# this can be downloaded from
#ftp://ftp.sanger.ac.uk/pub/databases/Pfam/current_release/
FULL_PFAM_PATH=/Users/kkreth/Never_Back_Up/Pfam-A.full

# where the COBS code is installed
COBS_HOME_DIRECTORY=d:\\KyleCleanroom

# files will be downloaded as needed via FTP from the PDB database and put in
this directory
PDB_DIR=d:\\pdbDir

# this file is included in the distribution
# it is based on part on
#ftp://ftp.sanger.ac.uk/pub/databases/Pfam/mappings/pdb_pfam_mapping.txt
#but includes additional information from the PFAM database
PDB_PFAM_CHAIN=D:\\KyleCodeRelease\\src\\bestPfamLines_pfamToPDB.txt

# these are where the result files will be held
COBS_CLEANROOM=D:\\COBS_OUT
```

Once this is setup run:

```
java -Xms1G -Xmx2G averagesAndOutput.WriteScores
```

If all has gone well in the COBS_CLEANROOM directory you should see a score file for each family and each score as well as the following summary files:

bigSummaries – A collapse of the scores from the results directory. It is here that any "normalization" using the APC method from Gloor can be used on any of the result files. Class: averagesAndOutput.AbsoluteScoreVsAverageDistance

Roc – Results for generating ROC files are placed, which perform the Cb to Cb 50th percentile cutoff calculation as discussed in the paper.
Class: averagesAndOutput.RocOnBigTable