for the accurate screened interaction and fragment desolvation
energies.

Files modified:
source/main.c
source/solv_frag.c
source/solv_lookup.c
source/funct.h
source/reinfi.c
inputs/seed.par

New documentation:
doc.ps

SEED 3.1 Release May 26, 2004

The following is introduced after the SEED 3.0 release dated
March 5, 2003.

1. Reduction of the number of output files
   Name : Nicolas Majeux
   Email address : majeux@bioc.unizh.ch
   Institution : Department of Biochemistry
   University of Zurich
   Date : May 26, 2004

The following files are not written out any more if the
"postprocess scheme" is selected: FragmentName_xxx.mol2,
FragmentName.chm, FragmentName_clus.chm, FragmentName_clus_reduc.chm .

File modified:
source/main.c

New documentation:
doc.ps

SEED 3.2 Release June 24, 2004

The following is introduced after the SEED 3.1 release dated
May 26, 2004.

1. Calculation of geometrical centers for FFLD
   Name : Nicolas Majeux
   Email address : majeux@bioc.unizh.ch
   Institution : Department of Biochemistry
   University of Zurich
   Date : June 24, 2004

The geometrical centers for FFLD are written out in
FragmentName_geomcent.mol2 files. The method is described
on page 413 of
M Cecchini, P Kolb, N Majeux, A Caflisch, Journal of Computational
Chemistry, 25, pp. 412–422, 2004.
Also on page 24 of the corresponding SEED documentation.

Files modified:
source/main.c
source/reinfi.c
source/funct.h
inputs/seed.par

File added: