XDRF2PDB, XDRF2PDB-M, XDRF2X
Programs to convert compressed Cartesian coordinate files from UNRES into ASCII formats

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2 PROGRAMS AND THEIR FUNCTONS

The following three programs can be used to extract conformations from compressed Cartesian (cx) files from UNRES:

xdrf2pdb — takes a single trajectory file and converts it into PDB format.

xdrf2pdb-m – takes a multiple-trajectory file from UNRES/MREMD simulations and enables the user to extract conformation of a particular trajectory and save them to a PDB file.

xdrf2x – takes a single trajectory file and converts it into UNRES Cartesian coordinate (x) format.

xdrf2ang – takes a single trajectory file and calculates UNRES backbone angles (theta and gamma).

3 INSTALLATION

Run make all on your system to install all programs or make *program* to install a particular program. You might need to run make in the xdrf subdirectory beforehand or point to the xdrf library that is on another directory in the Makefile.

The programs compile on all known Fortran compilers, including gfortran. It is recommeded to use Cmake to install whole package; please see Installation Guide.

4 COMMAND LINE AND FILES

For xdrf2pdb and xdrf2pdb-m, you'll need to prepare the UNRES sequence file in either one- or three-letter code.

4.1 XDRF2PDB

Command line syntax:

xdrf2pdb one/three seqfile cxfile [freq] [start] [end] [pdbfile]

one or three indicates in what format the sequence will be read

seqfile – the file with the sequence:

- one-letter format: 80A1
- three-letter format: 20(A3,1X)

Note that the sequence must match exactly the UNRES sequence.

cxfile – full name of the trajectory file with compressed Cartesian coordinates.

freq (1) – conformation sampling frequency (each freq-th conformation will be saved to PBD file.

start (1) – the first conformation to be saved to PDB file.

end (1000000000) – the last conformation to be saved to PDB file.

pdbfile (cxfile with extension changed from cx to pdb) – the output PDB file.

4.2 XDRF2PDB-M

Command line syntax:

xdrf2pdb-m one/three seqfile cxfile [ntraj] [itraj] [pdbfile] [ifreq]

cxfile - the name of the compressed trajectory file from an UNRES/MREMD run carried out with TRAJ1FILE (conformations from all trajectories output to a single file).

ntraj (1) – number of trajectories in the multi-trajectory run.

itraj (1) – the number of trajectory to be extracted.

4.3 XDRF2X

Command line syntax:

xdrf2x cxfile [is] [ie] [freq] > x_file

The meaning of the the arguments is as in section 4.1; the conformations are output in UNRES Cartesian coordinate format to stdout.

4.4 XDRF2ANG

Command line syntax:

xdrf2ang one/three seqfile cxfile [freq] [start] [end] [angfile]

The meaning of the first six parameters is as in section 4.1 angfile is the name of the output angle file; is assigned cx file name with the cx extension changed to ang, if not present.

5 SUPPORT

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