

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

Laboratory of Molecular Modeling
Faculty of Chemistry
University of Gdansk
Sobieskiego 18
80-952 Gdansk, Poland

Scheraga Group
Baker Laboratory of Chemistry
and Chemical Biology
Cornell University
Ithaca, NY 14853-1301, USA

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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 recommended 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 PDB file.

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

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

pdfile (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] [pdfile] [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

Dr. Adam Liwo
Faculty of Chemistry, University of Gdansk
ul. Wita Stwosza 63, 80-308 Gdansk Poland.
phone: +48 58 523 5124
fax: +48 58 523 5012
e-mail: adam@sun1.chem.univ.gda.pl

Dr. Cezary Czaplewski
Faculty of Chemistry, University of Gdansk
ul. Wita Stwosza 63, 80-308 Gdansk Poland.
phone: +48 58 523 5126
fax: +48 58 523 5012
e-mail: cezary.czaplewski@ug.edu.pl

Prepared by Adam Liwo, 11/26/11

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