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SIMULAID: simulation setup and analysis utilities, written by Mihaly Mezei
Version 02/25/2022; Memory use=1287 Mb; Maximum number of input records=250000
M. Mezei, J. Comp. Chem., Vol 31, 2658-2668 (2010). DOI:10.1002/jcc.21551
NOTE: input prompts showing ? will yield an explanation by typing just a ?
NOTE: input prompts showing + will yield a tip by typing just a +
Conversion files found in directory /simulaid
WARNING: could not determine if this is a cluster headnode
         Functions requiring sizable CPU time should be run on a compute node

SELECT run type:
Print all menu and submenu <F>unctions - - - - - - - - - -  : f
Geometry <O>ptimization (orientation, smallest sphere) [3]  : o
<C>leanup (sort, renumber, regroup, round charges) - - - -  : c
<S>tructure file and type conversions [15] - - - - - - - -  : s
<T>rajectory file and type conversions [4] - - - - - - - -  : t
Atom <N>ame and residue name conversions [4] - - - - - - -  : n
Trajectory - str<U>cture file conversions (pack/unpack) [4] : u
Conformation <E>dit (trans/rot/cent/algn/add/del, etc.) [15]: e
<M>iscellaneous (seq, RTF, UHBD, tors., Amber sum, etc.)[7] : m
<A>nalyze (TRAJELIX, RMSD, H-bonds, CV, etc.) [17] - - - -  : a
Cluste<R> atoms or data defined by a distance matrix [2] -  : r
Make the input <P>redictable - - - - - - - - - - - - - - -  : p
Open <L>ogfile logging the keyboard inputs - - - - - - - -  : l
<Q>uit Simulaid  - - - - - - - - - - - - - - - - - - - - -  : q  l
"Open logfile logging the keyboard inputs" selected
Name of the log file=trj.inp
File trj.inp (formatted) opened on unit  45
Keyboard inputs will be logged in the file trj.inp
Do you want to make the quizzes predictable (y/n/?) [y]
Interactive quizzes will not depend on the data.
Default options will be used and a message will be printed

SELECT run type:
Print all menu and submenu <F>unctions - - - - - - - - - -  : f
Geometry <O>ptimization (orientation, smallest sphere) [3]  : o
<C>leanup (sort, renumber, regroup, round charges) - - - -  : c
<S>tructure file and type conversions [15] - - - - - - - -  : s
<T>rajectory file and type conversions [4] - - - - - - - -  : t
Atom <N>ame and residue name conversions [4] - - - - - - -  : n
Trajectory - str<U>cture file conversions (pack/unpack) [4] : u
Conformation <E>dit (trans/rot/cent/algn/add/del, etc.) [15]: e
<M>iscellaneous (seq, RTF, UHBD, tors., Amber sum, etc.)[7] : m
<A>nalyze (TRAJELIX, RMSD, H-bonds, CV, etc.) [17] - - - -  : a
Cluste<R> atoms or data defined by a distance matrix [2] -  : r
Make the input <P>redictable - - - - - - - - - - - - - - -  : p
Open <L>ogfile logging the keyboard inputs - - - - - - - -  : l
<Q>uit Simulaid  - - - - - - - - - - - - - - - - - - - - -  : q  t
"Trajectory file and type conversions [4]" selected

SELECT trajectory file format conversion type:
Convert trajectory to <C>harmm format  - - - - - - - - - -  : c
Convert trajectory to <A>mber format - - - - - - - - - - -  : a
Convert trajectory to <M>acromodel format  - - - - - - - -  : m
Convert trajectory to <X>cluster format  - - - - - - - - -  : x
<S>eparate GCE MMC trajectory into Amber trajectories  - -  : s
<Q>uit trajectory conversion - - - - - - - - - - - - - - -  : q
Help - - - - - - - - - - - - - - - - - - - - - - - - - - -  : ?  a
"Convert trajectory to amber format" selected
Name of the input STRUCTURE file=mcd.pdb
File mcd.pdb (formatted) opened on unit  10
The input format is established as PDB
The PDB format is found to be Brookhaven
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Is that OK (y/n) [y]
The input format is established as Brookh. PDB
Do you have charges in the temperature factor column (y/n) [n]

SELECT  input trajectory file format:
<C>harmm/NAMD (.DCD) - - - - - - - - - - - - - - - - - - - -  : c
<A>mber  - - - - - - - - - - - - - - - - - - - - - - - - - - -  : a
MMC Monte Car<L>o  - - - - - - - - - - - - - - - - - - - - -  : l
Macr<O>model - - - - - - - - - - - - - - - - - - - - - - - -  : o
Macromodel/<X>cluster  - - - - - - - - - - - - - - - - - - -  : x
Amber C<D>F  - - - - - - - - - - - - - - - - - - - - - - - -  : d  c
"Charmm/NAMD (.DCD)" selected
Do you want to change atomnames to Brookhaven form (y/n/?) [n]
Note: all heteroatoms will be kept and
      only the first of alternate records will be used
Do you want to read chemical symbols from col 77-78 (y/n) [y] n
TITLE MCD - Mast Cell Degranulating Peptide

SELECT MODEL record treatment:
<K>eep MODEL/ENDMDL records  - - - - - - - - - - - - - - - -  : k (default)
<D>elete MODEL/ENDMDL records  - - - - - - - - - - - - - - -  : d
Change ENDMDL to <E>ND and delete MODEL records  - - - - - -  : e
Change ENDMDL to <T>ER and delete MODEL records  - - - - - -  : t
"Keep MODEL/ENDMDL records" selected
REMARK A. Buku, I. Keselman, D. Lupyan, M. Mezei and J.A. Price,
REMARK Chem. Biol. Drug Des, 72, 13-139 (2008).
REMARK DOI:10.1111/j.1747-0285.2008.00684.x
Atom name starting with two upper-case charcters(HG) found
Are both characters part of the chemical symbol (y/n) [n] n
Number of atoms found in the input file=    378
Title read:
MCD - Mast Cell Degranulating Peptide
Do you want to replace the title (y/n/+) [n]
Solvent residue name in the input file [HOH]=
Number of solute atoms found=         378
NOTE: no solvent residue HOH was found
Number of residues=          22  solute residues=          22
NOTE: residue numbers are not consecutive
Number of hydrogens in the solute=         200
There are   108 backbone atoms and     270 putative side chain solute atoms
 1    A      1-   378 Resid    1-   22 Resix    1-   22 MW=   2595 <B>=    0.0
For the purpose of PBC recentering small(er) molecules and ions
should be treated as solvents while the larger solute molecules
should be kept in their relative positions under PBC resets
If segments of the solute contains such molecules or ions those residues
have to be treated as separate molecules.
NOTE: segments of molecular residues should follow the segments to be
kept together
NOTE: trajectory conversion with Simulaid has an option to rearrange the atoms
Do you have molecular residues (e.g., ions) in this system (y/n/?) [n]
The solute contains   22 amino acid residues   0 nucleic acid residues
and     0 unclassified residues
The volume of the solute is estimated to be    3281.29 A^3
Volume of the protein (part) is estimated to be     3281.29 A^3
Dimensions of the solute:
Smallest, middle and largest X coordinate values= -10.8400  -0.2500  10.3400
Smallest, middle and largest Y coordinate values= -12.8900  -1.6750   9.5400
Smallest, middle and largest Z coordinate values= -10.7070   0.8710  12.4490
Volume of enclosing rectangle=    11000.66 A^3


SELECT Bond information source:
<C>oordinates of the input structure - - - - - - - - - - -  : c (default)
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User-supplied Charmm <P>SF file (Xplor format) - - - - - -  : p
User-supplied Amber <T>op file - - - - - - - - - - - - - -  : t  c
"Coordinates of the input structure" selected
Do you want to change bond thresholds (y/n/+) [n]
   21 chiral CAs were found,    21 in L and     0 in D conformation
    1 achiral CAs were found (glycine)
Name of the input trajectory file=mcd.dcd
File mcd.dcd (unformatted) opened on unit  70
Trajectory written by VMD
Number of data sets:     201
Number of free atoms=    378 Number of fixed atoms=      0
Charmm version=  24
Initial PBC box size information:   38.550762   38.886002   39.042850
Initial PBC box angle/cos information:    0.000000    0.000000    0.000000
Cell information is read for each configuration
Charmm-DCD  trajectory file mcd.dcd opened
Title:
Created by DCD plugin
REMARKS Created 28 January, 2008 at 16:59
Do you have a list of configurations to read (y/n) [n]
First structure to use from trajectory [ 1]=
Last  structure to use from trajectory [ 201]=
Increment [ 1,?]=
Number of configurations to use=         201

SELECT output atom order:
Leave the order <U>nchanged  - - - - - - - - - - - - - - - -  : u (default)
<R>ead the new order from a file (.sort, Charmm CRD or PDB) : r
Rearrange atoms by matching names to a <D>ifferent structure: d
Help - - - - - - - - - - - - - - - - - - - - - - - - - - - -  : ?
"Leave the order unchanged" selected
Do you want to select atoms to write (y/n) [n]
Periodic cell information was found
Do you want to override the cell size/shape (y/n) [n]

SELECT PBC cell type:
<N>o PBC - - - - - - - - - - - - - - - - - - - - - - - - - -  : n
<C>ubic  - - - - - - - - - - - - - - - - - - - - - - - - - -  : c
<R>ectangular  - - - - - - - - - - - - - - - - - - - - - - -  : r (default)
<F>ace-centered cubic  - - - - - - - - - - - - - - - - - - -  : f
<H>exagonal prism  - - - - - - - - - - - - - - - - - - - - -  : h
Ske<W>ed hexagonal prism - - - - - - - - - - - - - - - - - -  : w
<T>runcated octahedron, X -> square (Charmm) - - - - - - -  : t
Truncated <O>ctahedron, X -> hexagon (Amber, NAMD) - - - -  : o
He<X>agonal close-packed - - - - - - - - - - - - - - - - -  : x
Octahe<D>ral (NAMD)  - - - - - - - - - - - - - - - - - - -  : d
<I>mage file defined - - - - - - - - - - - - - - - - - - -  : i
<S>phere - - - - - - - - - - - - - - - - - - - - - - - - -  : s  r
"Rectangular" selected
Cell parameters are set from the trajectory to
 38.55076  38.88600  39.04285
Do you want to rotate each snapshot of the trajectory (y/n/?) [n]
Do you want to superimpose each frame to the input structure (y/n/+) [n]
Do you want to reset all molecules into the PBC cell (y/n) [y] n
Do you want to shift the origin to the box corner (y/n) [y] n
Name of the output trajectory file=mcd.trj
Opening file mcd.trj
If the file exists, do you want to overwrite it (y/n) [n] y
File mcd.trj (formatted) opened on unit  71
Current structure title:
MCD - Mast Cell Degranulating Peptide
Current trajectory title:
Created by DCD plugin
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Do you want to use the structure title for both (y/n) [y] y
First frame topology and solvent PBC checks passed
Do you want repeated box information (y/n/?/+) [y]
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