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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=dss.inp
File dss.inp (formatted) opened on unit  45
Keyboard inputs will be logged in the file dss.inp
Do you want to make the quizzes predictable (y/n/?) [y] 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  a
"Analyze (TRAJELIX, RMSD, H-bonds, CV, etc.) [17]" 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
Is that OK (y/n) [y] y
The input format is established as Brookh. PDB
Do you have charges in the temperature factor column (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)
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<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  k
"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]
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
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 configuration analysis:
<G>eometry/topology (links, bond, angle, torsion, etc.)  [4]: g
<B>ond (salt bridge, hydrogen/hydrophobic) track, corr.  [6]: b
Atomic propert<Y> (CV, hydrophobicity, Delphi potential) [3]: y
M<O>lecular property (shell vol, rad, com, dipole, axis) [4]: o
R<M>SD calculation (1D, 2D RMSD map, 2-traj cross RMSD)  [4]: m
Meas<U>re distances (atom-atom, residue-residue, etc.)   [8]: u
Plot PBC cell si<Z>es, volume  - - - - - - - - - - - - - -  : z
Psi-Phi R<A>machandran and dial plots  - - - - - - - - - -  : a
Bond angle statistics d<I>al plots - - - - - - - - - - - -  : i
<T>orsion angle statistics and dial plots  - - - - - - - -  : t
Proline <K>ink calculation - - - - - - - - - - - - - - - -  : k
Heli<X> analysis (TRAJELIX)  - - - - - - - - - - - - - - -  : x
<P>seudorotation angle calculation - - - - - - - - - - - -  : p
D<S>SP secondary structure assignment  - - - - - - - - - -  : s
Circular <V>ariance map  - - - - - - - - - - - - - - - - -  : v
Residue cov/cor matrix (from inp/traj), <N>ormal mode anal. : n
Summarize Amber energy <D>ecomposition tables (old format)  : d
<F>ilter solvents by solute distance and/or CV; by interface: f
<Q>uit analyzing this structure  - - - - - - - - - - - - -  : q  s
"DSSP secondary structure assignment" selected
Analysis selected: DSSP secondary structure assignment

SELECT Bond information source:
<C>oordinates of the input structure - - - - - - - - - - -  : c (default)
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]
Do you want to analyze a trajectory (y/n/+) [y]
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SELECT trajectory unit:
Number of <F>rames - - - - - - - - - - - - - - - - - - - - -  : f (default)
<P>icoseconds  - - - - - - - - - - - - - - - - - - - - - - -  : p
<N>anoseconds  - - - - - - - - - - - - - - - - - - - - - - -  : n
<M>iliseconds  - - - - - - - - - - - - - - - - - - - - - - -  : m  f
"Number of frames" selected
Opening file mcd.dss
If the file exists, do you want to overwrite it (y/n) [n] y
File mcd.dss (formatted) opened on unit  40
SIMULAID Version: 02/25/2022
Secondary structure assignment according to DSSP will be written to file
    mcd.dss
Secondary structure plot will be written to file

First residue sequence number to plot [ 1]=
Last  residue sequence number to plot [ 22]=
Actual residue number of the first residue=     1
Actual residue number of the last  residue=    22
Do you want to use the actual residue # on the Y axis (y/n) [n] y
Do you want to calculate turn information (see GW Rose) (y/n) [n]
Opening file mcd.dss.ps
If the file exists, do you want to overwrite it (y/n) [n] y
File mcd.dss.ps (formatted) opened on unit  50

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
Name of the 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

NOTE: warnings, summaries (if any) will be turned off after the 10-th frame
Start scan nmc=           0
First frame topology and solvent PBC checks passed
Could not generate H for residue           1

SS#  1 Residue index range: [   12,   19] Type:4-helix
Trajectory scan  10% done  Nframe=     20
Trajectory scan  20% done  Nframe=     40
Trajectory scan  30% done  Nframe=     60
Trajectory scan  40% done  Nframe=     80
Trajectory scan  50% done  Nframe=    100
Trajectory scan  60% done  Nframe=    120
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Trajectory scan  70% done  Nframe=    140
Trajectory scan  80% done  Nframe=    160
Trajectory scan  90% done  Nframe=    180

SELECT configuration analysis:
<G>eometry/topology (links, bond, angle, torsion, etc.)  [4]: g
<B>ond (salt bridge, hydrogen/hydrophobic) track, corr.  [6]: b
Atomic propert<Y> (CV, hydrophobicity, Delphi potential) [3]: y
M<O>lecular property (shell vol, rad, com, dipole, axis) [4]: o
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Psi-Phi R<A>machandran and dial plots  - - - - - - - - - -  : a
Bond angle statistics d<I>al plots - - - - - - - - - - - -  : i
<T>orsion angle statistics and dial plots  - - - - - - - -  : t
Proline <K>ink calculation - - - - - - - - - - - - - - - -  : k
Heli<X> analysis (TRAJELIX)  - - - - - - - - - - - - - - -  : x
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D<S>SP secondary structure assignment  - - - - - - - - - -  : s
Circular <V>ariance map  - - - - - - - - - - - - - - - - -  : v
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<Q>uit analyzing this structure  - - - - - - - - - - - - -  : q  q
"Quit analyzing this structure" selected
```