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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=hbn.inp
File hbn.inp (formatted) opened on unit  45
Keyboard inputs will be logged in the file hbn.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]
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]
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
"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
WARNING: column 77-78 is blank - atomic number will be deduced from atom name:
ATOM      1  N   ILE A   1      -9.986  -3.035   4.385  1.00  0.00
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  b
"Bond (salt bridge, hydrogen/hydrophobic) track, corr.  [6]" selected

SELECT bond tracking:
<H>ydrogen bond list, time course, and correlation - - - -  : h
Hydro<P>hobic contact list, time course, and correlation -  : p
<S>alt bridge list, time course, and correlation - - - - -  : s
Heavy atom VdW <C>ontact search  - - - - - - - - - - - - -  : c
M<U>tually proximal contact search - - - - - - - - - - - -  : u
Hydrogen-bonded <B>ridge search  - - - - - - - - - - - - -  : b
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Residue-residue bond (HB, SB or HPH) <M>atrix comparison -  : m
<Q>uit bond tracking - - - - - - - - - - - - - - - - - - -  : q  h
"Hydrogen bond list, time course, and correlation" selected
Analysis selected: Hydrogen-bond list

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] n
Do you want to analyze a trajectory (y/n/+) [y]

SELECT trajectory unit:
Number of <F>rames - - - - - - - - - - - - - - - - - - - -  : f (default)
<P>icoseconds  - - - - - - - - - - - - - - - - - - - - - -  : p
<N>anoseconds  - - - - - - - - - - - - - - - - - - - - - -  : n
<M>iliseconds  - - - - - - - - - - - - - - - - - - - - - -  : m  f
"Number of frames" selected

SELECT charge input:
<N>o charge input  - - - - - - - - - - - - - - - - - - - -  : n (default)
Input charges from <A>mber prmtop file - - - - - - - - - -  : a
Input charges from <C>harmm PSF file - - - - - - - - - - -  : c
Input charges from Auto<D>ock .pdbqt file  - - - - - - - -  : d
Input charges from <M>MC .slt file        `  - - - - - - -  : m  n
"No charge input" selected
NOTE: lack of charge information may hamper the bond definitions
      - you may want to consider other structure file formats
Run continues as predictable input was requested
Opening file mcd.hbn
If the file exists, do you want to overwrite it (y/n) [n] y
File mcd.hbn (formatted) opened on unit  40
SIMULAID Version: 02/25/2022
Do you want to calculate hydrogen bond correlation (y/n) [n]
Do you want to calculate residue-aggregated bond correlation (y/n) [n]
Do you want to print every hydrogen bond (y/n) [n]
Do you want to read previously generated bond tracks (y/n) [n]
Number of frames to average in the bond number plot [ 1]=
Hydrogen-bond list will be written to file
    mcd.hbn
H-bond length tolerance factor [ 1.50,?]=?
    H-bond A...H-D involves a threshold on the A - D distance
    it is calculated as the covalent bond threshold between
    atoms A and H times the tolerance factor
H-bond length tolerance factor [ 1.50,?]=
A-H...B angle minimum accepted [ 120.00,?]=?
    H-bond A...H-D involves a minimum value for the angle A-H-D
A-H...B angle minimum accepted [ 120.00,?]=
Potentially a hydrogen bond is formed between
  all  N atoms within  2.06 A of a hydrogen
  all  O atoms within  2.06 A of a hydrogen
  all  S atoms within  2.57 A of a hydrogen

SELECT Hydrogen bond hydrogen bond anchor atoms:
Use <A>ll qualifying atoms as potential anchors  - - - - -  : a
Give <L>ist of solute anchor atom indices  - - - - - - - -  : l
Specify a solute <S>egment (chain) - - - - - - - - - - -  : s
Give solute anchor atom inde<X> range  - - - - - - - - -  : x
Give list of solute anchor atom residue <N>umbers  - - - -  : n
Give solute anchor atom residue <R>ange  - - - - - - - - -  : r
Give list of solute anchor atom <T>ypes  - - - - - - - - -  : t
Use protein <B>ackbone O and H - - - - - - - - - - - - -  : b
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Use atoms with high enough partial <C>harge  - - - - - - -  : c
<Q>uit anchor definiton quiz - - - - - - - - - - - - - - -  : q
Help - - - - - - - - - - - - - - - - - - - - - - - - - - -  : ?  a
"Use all qualifying atoms as potential anchors" selected

SELECT Hydrogen bond hydrogen bond anchor atoms:
Use <A>ll qualifying atoms as potential anchors  - - - - -  : a
Give <L>ist of solute anchor atom indices  - - - - - - - -  : l
Specify a solute <S>egment (chain) - - - - - - - - - - -  : s
Give solute anchor atom inde<X> range  - - - - - - - - - -  : x
Give list of solute anchor atom residue <N>umbers  - - - -  : n
Give solute anchor atom residue <R>ange  - - - - - - - - -  : r
Give list of solute anchor atom <T>ypes  - - - - - - - - -  : t
Use protein <B>ackbone O and H - - - - - - - - - - - - - -  : b
Use atoms with high enough partial <C>harge  - - - - - - -  : c
<Q>uit anchor definiton quiz - - - - - - - - - - - - - - -  : q
Help - - - - - - - - - - - - - - - - - - - - - - - - - - -  : ?  q
"Quit anchor definiton quiz" selected
Do you want to omit protein backbone atoms (y/n) [n] n
Do you want to exclude intra segment/chain bonds (y/n) [n]
Number of carbons and aliphatic hydrogens filtered out=  254
Number of colors ( < 8)  [ 8,?]=?
    This input sets the number of different colors in the plots
Number of colors ( < 8)  [ 8,?]=5
Opening file mcd.hbn.ps
If the file exists, do you want to overwrite it (y/n) [n] y
File mcd.hbn.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
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
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Trajectory scan  60% done  Nframe=    120
Trajectory scan  70% done  Nframe=    140
Trajectory scan  80% done  Nframe=    160
Trajectory scan  90% done  Nframe=    180
Do you want to end the track statistics at the last on frame (y/n/?) [n]
Maximum number of hydrogen bonds=   13 at frame#      113
Number of hydrogen-bond types found=   51
Most persistent bond was present in    199 configurations
Number of anchor-anchor hydrogen bonds found=    51
Total number of hydrogen bonds / number of frames=    8.7
Histogram of the number of frames a bond is present over    201 configurations
(10% intervals of [    1 -   199] range:
    29      6      6      2      2      2      1      2      0      1
MINimum percentage presence [0.0,?]=10
MAXimum percentage presence [ 100.00,?]=
MINimum residue-residue sequence distance [ 1,?]=
MAXimum residue-residue sequence distance [ 21,?]=
Number of hydrogen bonds left after filtering=   20
Do you want to calculate bond autocorrelation (y/n) [n]
Do you want a list of bonded atom pairs (y/n/+) [n]
Do you want to limit the bond sums to the filtered bonds (y/n) [n]
Number of data points to average in the 1D plot(s) [ 1]=

Generating residue-contracted bond information
Do yo want to filter the residue-aggregated bonds (y/n/?) [y]
MINimum percentage presence [ 10.00,?]=
MAXimum percentage presence [ 100.00,?]=
MINimum residue-residue sequence distance [ 1,?]=
MAXimum residue-residue sequence distance [ 21,?]=
Number of residue-residue pairs filtered down from    16 to   33
After res-res filtering the number of hydrogen bonds
changed from    51 to   33
Number of residues involved in hydrogen bonding=   18
Do you want only hydrogen-bonded residues in the plot (y/n/?) [y] ?
    Yes answer will produce an smaller matrix. The actual
    residues corresponding to the matrix rows and colums are
    printed ont the .hbn file. No answer will plot a matrix with
    all residues.
Do you want only hydrogen-bonded residues in the plot (y/n/?) [y]

SELECT treatment of contacts:
Calculate <A>verage residue-residue contacts - - - - - - -  : a
Calculate <C>umulative contacts  - - - - - - - - - - - - -  : c (default)
<I>gnore multiple contacts - - - - - - - - - - - - - - - -  : i
Help - - - - - - - - - - - - - - - - - - - - - - - - - - -  : ?  ?
    This question settles the treatment of more than one
    hydrogen or hydrophobic bonds between some residue pairs.
    Asking for averaging will calculate the bond fractions as
    the total number of bonds divided by the number of frames
    and by the number of possible bonds between this residue
    pair. Asking for cumulative averaging will result in
    dividing by the number of frames only. Asking for ignoring
    multiple contacts will just average the number of times this
    residue pair was in contact through any of the possible
    bonds.

SELECT treatment of contacts:
Calculate <A>verage residue-residue contacts - - - - - - -  : a
Calculate <C>umulative contacts  - - - - - - - - - - - - -  : c (default)
<I>gnore multiple contacts - - - - - - - - - - - - - - - -  : i
Help - - - - - - - - - - - - - - - - - - - - - - - - - - -  : ?  c
"Calculate cumulative contacts" selected
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Maximum number of hydrogen bonds between two residues=   6
Limit of the residue-residue hydrogen bond map [ 0.99005,?]=
Last residue to plot on the Y axis [ 18,?]=
First residue to plot on the Y axis [ 1,?]=
Do you want to calculate residue-residue autocorrelation (y/n) [n]
Do you want to write the bond tracks (y/n/+) [n] +
    Bond tracks are useful for reanalyzing different segments of
    the run or repeating the residence time calculation via
    autocorrelation
Do you want to write the bond tracks (y/n/+) [n]
Current structure is the input structure
Do you want a PDB file of the current structure with % bonds (y/n) [n] y
Do you want to add lines between the residue pairs (y/n/?) [n] y
Do you want percentages added to all atoms in a residue (y/n/?) [n]
Opening file mcd.pcb.pdb
If the file exists, do you want to overwrite it (y/n) [n] y
File mcd.pcb.pdb (formatted) opened on unit  44

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  q
"Quit analyzing this structure" selected
```