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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=rgh.inp
File rgh.inp (formatted) opened on unit  45
Keyboard inputs will be logged in the file rgh.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
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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  o
"Molecular property (shell vol, rad, com, dipole, axis) [4]" selected

SELECT molecular property calculation:
S<O>lvation shell volume - - - - - - - - - - - - - - - - -  : o
Principal axis <D>irections and alignment  - - - - - - - -  : d
Radius (gyration, hydrodynamic), COM, inert, dipole <M>oment: m
Membrane <F>latness calculation  - - - - - - - - - - - - -  : f
<Q>uit molecular property calculation  - - - - - - - - - -  : q
Help - - - - - - - - - - - - - - - - - - - - - - - - - - -  : ?  m
"Radius (gyration, hydrodynamic), COM, inert, dipole moment" selected
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Analysis selected: Radius and dipole calculation

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/+) [n] y

SELECT trajectory unit:
Number of <F>rames - - - - - - - - - - - - - - - - - - - -  : f (default)
<P>icoseconds  - - - - - - - - - - - - - - - - - - - - - -  : p
<N>anoseconds  - - - - - - - - - - - - - - - - - - - - - -  : n
<M>iliseconds  - - - - - - - - - - - - - - - - - - - - - -  : m
"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
Do you want to rotate each frame of the trajectory (y/n) [n]
Opening file mcd.rgh
If the file exists, do you want to overwrite it (y/n) [n] y
SIMULAID Version: 02/25/2022
Select the atoms for the calculation
Selecting atoms from the system
Number of solute atoms=   378 Largest solute residue number=    22

SELECT selecting option:
Keep all solute atoms - i.e., drop sol<V>ents (if any) - -  : v
Select (keep only one) <C>hain/segment/molecule (id) - - -  : c
Excise (drop only one) chain/<S>egment/molecule (id) - - -  : s
Keep only the <B>ackbone - - - - - - - - - - - - - - - - -  : b
Keep only the <A>lpha carbons  - - - - - - - - - - - - - -  : a
Drop aliphatic <H>ydrogens - - - - - - - - - - - - - - - -  : h
Drop al<L> hydrogens - - - - - - - - - - - - - - - - - - -  : l
Select atom range to <K>eep  - - - - - - - - - - - - - - -  : k
Select atom range to <D>rop  - - - - - - - - - - - - - - -  : d
Select <R>esidue index range to keep - - - - - - - - - - -  : r
Select r<E>sidue index range to drop - - - - - - - - - - -  : e
Select a<T>om names to keep  - - - - - - - - - - - - - - -  : t
Select resid<U>e names to keep - - - - - - - - - - - - - -  : u
<Q>uit selecting - - - - - - - - - - - - - - - - - - - - -  : q  v
"Keep all solute atoms - i.e., drop solvents (if any)" selected
There are no solvents in the system - check the solvent residue name
          0  atoms deleted in this step

SELECT selecting option:
Keep all solute atoms - i.e., drop sol<V>ents (if any) - -  : v
Select (keep only one) <C>hain/segment/molecule (id) - - -  : c
Excise (drop only one) chain/<S>egment/molecule (id) - - -  : s
Keep only the <B>ackbone - - - - - - - - - - - - - - - - -  : b
Keep only the <A>lpha carbons  - - - - - - - - - - - - - -  : a
Drop aliphatic <H>ydrogens - - - - - - - - - - - - - - - -  : h
Drop al<L> hydrogens - - - - - - - - - - - - - - - - - - -  : l
Select atom range to <K>eep  - - - - - - - - - - - - - - -  : k
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```
Select atom range to <D>rop  - - - - - - - - - - - - - - - - - - - -  : d
Select <R>esidue index range to keep - - - - - - - - - - - - - - - -  : r
Select r<E>sidue index range to drop - - - - - - - - - - - - - - - -  : e
Select a<T>om names to keep  - - - - - - - - - - - - - - - - - - - -  : t
Select resid<U>e names to keep - - - - - - - - - - - - - - - - - - -  : u
<Q>uit selecting - - - - - - - - - - - - - - - - - - - - - - - - - -  : q  q
"Quit selecting" selected
Calculation of radii of gyration, hydrodynamic radius  moments of inertia and
(when charges are available) and dipole moment
Atoms used: 1-378
Radius of gyration, hydrodynamic radius moments of inertia
and (if charges are available) dipole moment will be written to file
mcd.rgh
Evolution and distribution plots will be written to file

Do you want mass-weighting (y/n) [y]
Opening file mcd.rgh.ps
If the file exists, do you want to overwrite it (y/n) [n] y
File mcd.rgh.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  a
"Amber" selected
Name of the trajectory file=mcd.trj
File mcd.trj (formatted) opened on unit  70
Opening Amber trajectory, number of atoms per structure=     378
Amber trajectory file title:
MCD - Mast Cell Degranulating Peptide
Box information was found after each structure
Amber-crd   trajectory file mcd.trj opened
Title:
MCD - Mast Cell Degranulating Peptide
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
Trajectory scan  60% done  Nframe=    120
Trajectory scan  70% done  Nframe=    140
Trajectory scan  80% done  Nframe=    160
Trajectory scan  90% done  Nframe=    180
Number of data points to average in the 1D plot(s) [ 1]=
The Postscript plots will be written to the file
mcd.rgh.ps

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
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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
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<T>orsion angle statistics and dial plots  - - - - - - - -  : t
Proline <K>ink calculation - - - - - - - - - - - - - - - -  : k
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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
```