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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=ort.inp
 File ort.inp (formatted) opened on unit  45
 Keyboard inputs will be logged in the file ort.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  e
 "Conformation edit (trans/rot/cent/algn/add/del, etc.) [15]" selected

 SELECT conformation manipulation:
 <E>dit the configuration (delete selected atoms) - - - - -  : e
 <R>otate/translate/scale/center/seprate/swap chirality - -  : r
 Permute the xy<Z> coordinates of a structure - - - - - - -  : z
 Modif<Y> the configuration (mutate/add atoms)  - - - - - -  : y
 Replace coordi<N>ates of a configuration from an other conf.: n
 <O>verlay structure on a reference structure - - - - - - -  : o
 Change a peptide to re<T>ro-inverso  - - - - - - - - - - -  : t
 Replace c<H>arges of a configuration from an other conf. -  : h
 Write P<D>B file of the residue trace (alpha carbons)  - -  : d
 Fi<X> water geometry to experimental geometry  - - - - - -  : x
 Trim <W>aters outside a simulation cell  - - - - - - - - -  : w
 Re<V>erse a previous optimization  - - - - - - - - - - - -  : v
 Create full crystal <C>ell from the asymmetric unit  - - -  : c
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Create <B>iological oligomers from the asymmetric unit - -  : b
Gather all crysta<L> contacts of the asymmetric unit - - -  : l
Cre<A>te neighboring PBC cells - - - - - - - - - - - - - -  : a
<Q>uit conformation manipulation selection - - - - - - - -  : q  r
"Rotate/translate/scale/center/seprate/swap chirality" 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]
Name of the output file=mcd_ort.pdb
Opening file mcd_ort.pdb
If the file exists, do you want to overwrite it (y/n) [n] y
File mcd_ort.pdb (formatted) opened on unit  20
The output format is established as PDB
New file - Brookhaven PDB selected
The output format is established as Brookh. PDB
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]
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
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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)
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)

SELECT (additional) conformation transformation type:
<S>hift (translate) the system by an input vector  - - - -  : s
Shift the system to a new position of a selected <A>tom  -  : a
Shift the system and reset it into a <P>BC cell  - - - - -  : p
<C>enter the system in a PBC cell  - - - - - - - - - - - -  : c
S<H>ift the center of the system to <0,0,0>  - - - - - - -  : h
<R>otate the system by an angle  - - - - - - - - - - - - -  : r
Rotate the system based on <B>ond directions - - - - - - -  : b
Sca<L>e the coordinates (change units) - - - - - - - - - -  : l
S<E>parate molecules (for clarity) - - - - - - - - - - - -  : e
S<W>ap chirality - - - - - - - - - - - - - - - - - - - - -  : w
<Q>uit conformation transformation type selection  - - - -  : q  b
"Rotate the system based on bond directions" selected
Atom index to put at the origin [ 1]=
Atom index to put on the X axis [ 1]=10
Atom index to put in the X-Y plane [ 1]=20
Atom at the origin:  N   ILE    1
Atom on the X axis: HG21 ILE    1
Atom in the X-Y plane:  C   ILE    1
System was rotated with the rotation matrix:
           0.2655959  0.9132942 -0.3087922
           0.6637517 -0.4055203 -0.6284798
          -0.6992085 -0.0380397 -0.7139051

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<R>otate the system by an angle  - - - - - - - - - - - - -  : r
Rotate the system based on <B>ond directions - - - - - - -  : b
Sca<L>e the coordinates (change units) - - - - - - - - - -  : l
S<E>parate molecules (for clarity) - - - - - - - - - - - -  : e
S<W>ap chirality - - - - - - - - - - - - - - - - - - - - -  : w
<Q>uit conformation transformation type selection  - - - -  : q  q
"Quit conformation transformation type selection" selected
Do you want chemical names written in the PDB file (y/n) [n]
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