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SIMULAID: simulation setup and analysis utilities, written by Mihaly Mezei
 Version 03/04/2023; Memory use=1288 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
 Eigen<V>alue/eigenvector calculation from input matrix (NMA): v
 Make the input <P>redictable - - - - - - - - - - - - - - -  : p
 Open <L>ogfile logging the keyboard inputs - - - - - - - -  : l
 <Q>uit Simulaid  - - - - - - - - - - - - - - - - - - - - -  : q  p
 "Make the input predictable" selected
 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
 Eigen<V>alue/eigenvector calculation from input matrix (NMA): v
 Make the input <P>redictable - - - - - - - - - - - - - - -  : p
 Open <L>ogfile logging the keyboard inputs - - - - - - - -  : l
 <Q>uit Simulaid  - - - - - - - - - - - - - - - - - - - - -  : q  B
 "Structure file and type conversions [15]" selected

 SELECT structure file format conversion type:
 Rearrange a<T>oms in a structure ccording to an RTF file -  : t
 Convert structure to <C>harmm CRD format - - - - - - - - -  : c
 Convert structure to <E>xtended Charmm CRD format  - - - -  : e
 Convert structure to Brookhaven <P>DB format - - - - - - -  : p
 Convert structure to C<H>armm PDB format (seg id)  - - - -  : h
 Convert structure to <M>acromodel dat format - - - - - - -  : m
 Convert structure to MMC Monte Car<L>o input - - - - - - -  : l
 Convert structure to <G>romos/Gromacs format - - - - - - -  : g
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Convert structure to <I>nsightII .car format - - - - - - -  : i
Convert structure to InsightII <N>xyz free format  - - - -  : n
Convert structure to InsightII <S>xyz free format  - - - -  : s
Convert structure to InsightII sxyz<R>q free form. - - - -  : r
Convert structure to <A>msol 3.5 input format  - - - - - -  : a
Convert structure to Gaussian <O>niom format - - - - - - -  : o
List column ranges for a different structure <F>ormat  - -  : f
<Q>uit structure file format conversion  - - - - - - - - -  : q  B
"Convert structure to Brookhaven PDB format" selected
Name of the input STRUCTURE file=mcd.mae
File mcd.mae (formatted) opened on unit  10
The input format is established as SCH Maestro
Output file name: mcd.pdb  - is it OK (y/n) [y] n
Name of the output file=mcd_cnv.pdb
Opening file mcd_cnv.pdb
If the file exists, do you want to overwrite it (y/n) [n] y
NOTE: atomnames, potential types are the chemical names
Do you want to change atomnames to Brookhaven form (y/n/?) [n] n
NOTE: This format is for input only
Number of atoms found in the input file=    380
Title read:
"- Mast Cell Degranulating Peptide"
Do you want to replace the title (y/n/+) [n] n
Solvent residue name in the input file [HOH     ]=HOH
Number of solute atoms found=         380
NOTE: no solvent residue HOH      was found
Number of residues=          28  solute residues=          28
NOTE: residue numbers are not consecutive
Number of hydrogens in the solute=         202
There are   108 backbone atoms and     272 putative side chain solute atoms
 1           1-   380 Resid    1-   14 Resix    1-   28 MW=   2597 qsm=   10.00
The solute contains   28 amino acid residues   0 nucleic acid residues
and     0 unclassified residues
The volume of the solute is estimated to be    4226.31 A^3
Volume of the protein (part) is estimated to be     4226.31 A^3
Dimensions of the solute:
Smallest, middle and largest X coordinate values= -10.9520  -0.3247  10.3025
Smallest, middle and largest Y coordinate values= -13.1664  -1.7256   9.7152
Smallest, middle and largest Z coordinate values= -10.8275   0.7824  12.3922
Volume of enclosing rectangle=    11292.64 A^3
Minimum deviation from integral residue charge to print [0.0]=0.0
Charge sum on residue     7 (7      ARG     ) is not integer:    0.9400
Charge sum on residue     8 (8      HSE     ) is not integer:   -0.6300
Charge sum on residue     9 (9      VAL     ) is not integer:   -0.3600
Charge sum on residue    12 (12     PRO     ) is not integer:   -0.0600
Charge sum on residue    13 (13     HSE     ) is not integer:   -0.6300
Charge sum on residue    14 (14     ILE     ) is not integer:   -0.3600
Charge sum on residue     7 (7      ARG     ) is not integer:    0.0600
Charge sum on residue     8 (8      HSE     ) is not integer:    1.6300
Charge sum on residue     9 (9      VAL     ) is not integer:    0.3600
Charge sum on residue    12 (12     PRO     ) is not integer:    0.0600
Charge sum on residue    13 (13     HSE     ) is not integer:    1.6300
Charge sum on residue    14 (14     ILE     ) is not integer:    0.3600
Checked     28 residues for charge sum. Total charge=   9.99998 e
Number of residues with nonintegral charge sum=  12
Charged residues (residues with nonintegral charges omitted):
   1(ILE     )    2(LYS     )    6(LYS     )   11(LYS     )   16(ARG     )
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  17(LYS     )   21(LYS     )
Largest absolute deviation from integral charge= 0.37000
Do you want to redistribute charges to integral resid sums (y/n/?) [n] n
Center-of-mass=    0.2634   -0.1302    0.2799 A
Dipole moment of the solute=    23.021
Dipole moment vector of solute =   -18.442    -8.237   -11.046 au*A

   21 chiral CAs were found,    21 in L and     0 in D conformation
    6 achiral CAs were found (glycine)
Do you want to sort the atoms (y/n) [n] y
Do you want chemical names written in the PDB file (y/n) [n] n
NOTE: This conversion only affects the record format.
    Atom and residue names are changed with the conversion option
    "converting to di<F>ferent PDB residue and atomname convention"
Do you want topology file based CONECT records (y/n) [n] n
Sorting by segment (chain) id and residue id
Do you want to adjust atom and residue numbers (y/n) [y] y
Atom number of the first atom [ 1,?]=1
Residue number of the first residue [ 1,?]=1
Do you want to restart residue numbering at each segment (y/n) [n] n
Atom and/or residue sequence numbers were changed
Do you want a sequence list (y/n) [n] n
NOTE: segment IDs are reduced to 1 character
NOTE: induced-fit poses are saved as separate full configurations
Total number of additional configurations to process [ 0,?]=0
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