

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/align/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 1
"Open logfile logging the keyboard inputs" selected
Name of the log file=axd.inp
File axd.inp (formatted) opened on unit 45
Keyboard inputs will be logged in the file axd.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
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<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] n
TITLE MCD - Mast Cell Degranulating Peptide
```

SELECT MODEL record treatment:

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<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. Lupyman, 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:

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<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 x
"Helix analysis (TRAJELIX)" selected
Analysis selected: Helix axis directions

```

SELECT Bond information source:

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<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

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SELECT trajectory unit:
Number of <F>frames - - - - - : f (default)
<P>icoseconds - - - - - : p
<N>anoseconds - - - - - : n
<M>iliseconds - - - - - : m
"Number of frames" selected
Do you want to rotate each frame of the trajectory (y/n) [n]
Opening file mcd.axd
If the file exists, do you want to overwrite it (y/n) [n] y
File mcd.axd (formatted) opened on unit 40
SIMULAID Version: 02/25/2022
Do you want to calculate angle probability distributions (y/n) [y]
Angle distribution grid size [ 2]=
Do you want to map the angle distributions on the dials (y/n) [y]
Do you want to draw arcs in the dial plots (y/n) [y]
Number of helices to analyze [ 1]=
NOTE: residue numbers refer to the actual residue number in the input structure
First helix residue=13
Last helix residue=19

```

Backbone	rn=	13	res=HSE	13	Atnos for CA, C, N=	214	227	212
Backbone	rn=	14	res=ILE	14	Atnos for CA, C, N=	231	246	229
Backbone	rn=	15	res=CYS	15	Atnos for CA, C, N=	252	256	250
Backbone	rn=	16	res=ARG	16	Atnos for CA, C, N=	260	280	258
Backbone	rn=	17	res=LYS	17	Atnos for CA, C, N=	284	302	282
Backbone	rn=	18	res=ILE	18	Atnos for CA, C, N=	306	321	304
Backbone	rn=	19	res=CYS	19	Atnos for CA, C, N=	327	331	325

```

Number of residues to ignore for rotation at each end [ 0]=
Is this a transmembrane protein (y/n) [n]
Do you want debug output (y/n) [n]
Minimum distance (in A) from axis to count as bend [0.0]=
Do you want to subtract the solute COM shift from the helix shift (y/n) [y]
Do you want to overlay each frame on the reference structure (y/n/+) [y]
Do you want to run DSSP check on each frame (y/n) [y]
Do you want mass-weighting (y/n) [y]
Opening file mcd.axd.ps
If the file exists, do you want to overwrite it (y/n) [n] y
File mcd.axd.ps (formatted) opened on unit 50

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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

Helix 1 direction established from the reference structure as the X axis

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
Reference helix # 1 is intact: HHHHHHH

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

Drawing 6 dials for 201 frames

Number of snapshots to average in the dials [1,?]=

Number of intact helices: 138
Number of broken helices: 0
Number of frayed helices: 63

Global helix X tilt-angle average= 26.64 CV= 0.00220
Global helix Y-tilt angle average= 114.30 CV= 0.00161
Global helix Z-tilt angle average= 80.43 CV= 0.00244

Helix rotation average= 2.40 CV= 0.00628

Local helix tilt average= 10.83 CV= 0.00217

Turn angle per res. average= 99.05 CV= 0.00044

Helix length average= 9.47 S.D.= 0.34

Curvature radius average= 6.33 S.D.= 0.28

Total displacement (cent) average= 0.84 S.D.= 0.24

X-displacement (cent) average= -0.60 S.D.= 0.28

Y-displacement (cent) average= -0.22 S.D.= 0.18

Z-displacement (cent) average= -0.42 S.D.= 0.25

Y-displacement (start) average= 0.58 S.D.= 0.37

Z-displacement (start) average= -0.91 S.D.= 0.46

Y-displacement (end) average= -0.88 S.D.= 0.31

Z-displacement (end) average= -0.06 S.D.= 0.36

Number of data points to average in the 1D plot(s) [1]=

Number of snapshots to average in the 2D tr [1,?]=

The Postscript plots will be written to the file
mcd.axd.ps

SELECT configuration analysis:

<G>eometry/topology (links, bond, angle, torsion, etc.)	[4]: g
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
```