Supplementary Materials

Table 1S. Time-dependent properties in CORREL.

Energy or geometry of bonds, angles or torsion angles
Axis of a helix that fits the specified set of atoms
3-dimensional vectors, their individual components or lengths, defined by atom positions or differences between sets of atom positions
Fluctuations in vectors, components and lengths defined by atom positions
Scalar and cross products between vectors defined by atom positions or differences between sets of atom positions
Principal moments of inertia
Solvent accessible or contact surface area,[146] for all selected atoms, or on a per-residue basis
Energy and hydrogen bond properties
Radius of gyration
Temperature
Density within a given radius
Ring puckering
RMS deviation from a reference structure, with or without least-squares superposition
Dipole moment for selected atoms or for a solvent shell of specified thickness
Scalar product of velocities or coordinate displacements with a previously determined normal mode of the system
Unit cell parameters

Time-dependent properties obtainable in an analysis of a trajectory using the CORREL module in CHARMM.

Table 2S. Coordinate Manipulation and Analysis Tools.

Manipulation Tools

ADD	Sum two coordinate sets.
AVERage	Generate an interpolated structure.
CONVert	Convert between fractional, symmetric, and aligned coordinates.
COPY	Copy coordinates from one set to another.
DIFFerence	Subtract two coordinate sets.
DRAW	Display a coordinate frame (if graphics is already activated).
DUPLicate	Copy coordinates from one set of atoms to another set.
DYNAmics	Get average coordinates and isotropic fluctuations from a trajectory.
FORCe	Copy forces to a coordinate set.
INITialize	Set coordinates to an initial, unused, value.
OPERate	Apply a specific symmetry transformation on selected atoms.
ORIEnt	Align atoms to the origin and rotate to best-fit the X-Y plane.
ORIEnt RMS	Best-fit one structure with another (minimizes RMS difference).
PAXAnalysis	Generate a principal axis analysis from atomic fluctuations.
ROTAte	Rotate selected atoms.
SCALe	Scale current data (often used with velocities).
SET	Set coordinate values to a constant.
SHAKe	Modify structures to conform to holonomic constraints.
SWAP	Exchange selected coordinates between sets.
TRANslate	Translate selected atoms.
TWISt	Twist (deform) about a chosen axis.

Analysis Tools

ANALysis	Accumulate solvent-averaged properties from dynamics.
AXIS	Generate an axis vector defined by one or two sets of atoms.
CONTact	Compute contact distance statistics from dynamics.
COVAriance	Calculate a covariance matrix from dynamic fluctuations.
DIPOle	Calculate the dipole moment (and other tensors).
DISTance	Calculate a distance matrix or vector for selected atoms.
DMAT	An alternate distance matrix analysis command.
HBONd	Compute hydrogen bond statistics from dynamics.
HELIx	Calculate an optimal helix or compare helices for two sets of atoms
HISTogram	Compute a histogram from a dynamic or a static structure.
INERtia	Calculate a moment of inertia tensor or rotational entropy.
LSQP	Calculate a least-squares plane for a selected set of atoms.
MINDist	Find the minimum distance between two sets of atoms.
MAXDist	Find the maximum distance between two sets of atoms.
PUCKer	Calculate a ring pucker for 5-member rings.
RGYR	Compute a radius of gyration.
RMS	Compute the RMS difference between atoms in two structures.

SEARch	Search for volume elements that are occupied, vacuum, or holes.
SECS	Secondary structure analysis of proteins.
STATistics	Compute simple statistics.
SURFace	Calculate surface areas using an analytic or grid based method.

CHARMM tools for manipulating and analyzing system coordinates (*COOR* command options; see "corman.doc").

Table 3S. Internal coordinate manipulation tools.

GENErate	Generate an IC table for selected atoms.
PARAmeters	Fill IC table with (default) angle and distance data from the parameter file.
FILL	Convert from Cartesian to internal coordinates.
DIFFerences	Compare two structures by calculating IC differences.
DERIvatives	Project forces or velocities into internal coordinate derivatives.
DYNAmics	Compute IC averages and fluctuations from dynamics.
EDIT	Edit elements of the IC table.
SEED	Initiate a build. Put 1st atom at the origin, 2nd on X-axis,…
BUILd	Convert from internal to Cartesian coordinates.
PURGe	Delete any partial IC elements.
ADD	Sum IC element values common to main and secondary tables.
SUBTract	Compute difference of IC element values common to both tables.
SCALe	Scale IC elements of selected table.
RANDom	Randomize selected torsion angles (for subsequent random build).
GAUSsian	Generate a special IC table for the Gaussian QM program.
PUCKer	Fill IC table elements with particular ring pucker values.
DELete	Delete IC elements containing unwanted atoms.
KEEP	Retain IC elements containing selected atoms (discarding remainder).
SAVE	Copy from main to secondary table.
RESTore	Copy from secondary to main table.
READ	Read IC table, with or without additional *APPEnd* option.
WRITe	Write IC table, with or without additional *RESI* (high precision) option.
PRINt	Print specified IC table.

Tools available in CHARMM (*IC* command options) for manipulating the internal coordinates of the system. See also "intcor.doc."