

Chime Rasmol Scripts

Tag name: **anim**

Description: Sets the animation mode, direction and speed. You can use either `anim` or `animation` as the command

Syntax:

```
anim {on|off|info}  
or  
anim mode {loop|once|palindrome}  
or  
anim direction {+1|-1}  
or  
anim fps ###  
or  
anim frame {next|-1|###}
```

You must specify one of the following settings. There is no default setting.

on - starts playing the animation

off - stops the animation

info - shows animation information (you can also use `show animation`)

mode - sets how the animation starts and ends. If you use `anim mode`, you must specify one of the following settings:

loop - loop from start to end and repeat

once - loop from start to end once

palindrome - loop start to end, then end to start, and repeat

direction - sets the current play direction. If you use `anim direction`, you must specify one of the following settings:

+1 - advances to the next animation frame in the current direction

-1 - moves to the previous frame

fps - frames per second. If you use `anim fps`, you must specify:

- number of frames per second

frame - sets which frame to be displayed. If you use `anim frame`, you must specify one of the following settings:

next - advances to the next animation frame in the current direction

-1 - moves to the previous frame

- jumps to the specified frame number

Tag name: **calculate charges**

Description: Specifies whether Chime should calculate atom charges. Charges are used to calculate potentials when showing MEP or MLP colors on a surface ("color list {listname} mep|mlp").

Syntax: `calculate charges {true|false|refresh}`
or `calc charges {true|false|refresh}`

true - (default) if charges are needed for potential calcs (MEP for example) then they WILL BE calculated if there is NO negative/positive temperature data in PDB file, or no charges in MOL, etc. file. (if there are negative values in PDB file charge data then Chime will not calculate charges by default. See "refresh" below for FORCING recalculation of charges).

false - Prevents Chime from recalculating charge data (and overwriting PDB file temperature data). This option allows the user to use any PDB file temperature data for MEP calcs.

refresh - Forces the recalculation of charges for the current structure. This can be useful for forcing the overwriting of PDB temperature data, or after a "set charge function" command.

Tag name: `center xyz`

Description: Sets the zoom/translate center to a specific point, rather than a specific atom

Syntax: `center xyz #x# #y# #z#`

#x# - the x coordinate.

#y# - the y coordinate.

#z# - the z coordinate.

Tag name: `color dots mep`

Description: Can be used color dots based on MEP calculations

Syntax: `color dots mep`

Tag name: `color list`

Description: Colors a surface using a specific type of mapping and specific colors

Syntax:

```

    color list {listname} [save] {list color command}
    or
    color list {listname} [colors] {list of colors only}
    or
    list {listname} color {list of colors only}

```

listname - name of the surface, assigned in the "surface", "load pmesh" or "load surface gaussian" command that creates the surface.

save - optional keyword that tells Chime not to recalculate the specified property if it has already been calculated, but to update the color map used for texturing. This can be much faster for experimenting with alternate coloring schemes.

colors - optional keyword indicating that what follows is a list of colors, not a color command.

The list color commands are as follows:

Command	Qualifier	Description
mep or potential		Color surface using Molecular Electrostatic Potential calculations. Up to 9 colors can be specified. If multiple colors are specified, they are used to represent different MEP energies along a continuum from lowest to highest. The special color <code>clear</code> or <code>transparent</code> denotes parts of the texture map that will not be rendered.
	rasmol	(optional) Use rasmol potential coloring scheme instead of default red-white-blue schema.
	iso	(optional) Use isocontour coloring scheme. This qualifier requires additional arguments, syntax: iso #number# [contourcolor maincolor lowestband_color highestband_color] If the #number# is an integer, then it specifies the number of contour lines over the whole range. If #number# has a decimal point, it specifies the size of the divisions between contour lines. The maincolor defaults to white, the contourcolor to black. The high/low colors, because they also default to white, do not appear.
mlp		Color list using Molecular Lipophilicity Potential calculations.
	See mep	The same qualifiers are used as in mep.
center		Color list based on distance from origin (center). If multiple colors are specified, they are used to represent different distances from shortest to longest.
distance	#distance#	Color list based the distance to the nearest selected atom divided by the specified distance. Anything near or greater than specified distance gets mapped to the last texture map color specified.
	see mep	The same optional qualifiers are used as in mep.
atom		Color list based on the closest atom's color. This can be used after the various atom/residue coloring commands to color the surface in interesting ways.

selected		Turn ON/OFF display of surface within/outside a specified distance from the nearest selected atom. Syntax: selected [distance] [within On Show Off Clear] [outside On Show Off Clear] For example, "color list test selected 6.0 on off" would turn the parts of surface "test" ON that are within 6.0 angstroms of the nearest selected atom, and the parts of the surface OFF that are outside that range.
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The default color scheme for a Gaillard MEP or MLP calculation is as follows:

Color	Actual Value	Normalized
Red	-infinity	-0.50 - -0.39
Purple		-0.39 - -0.28
Orange		-0.28 - -0.17
Yellow		-0.17 - -0.06
White	0	-0.06 - 0.06
Cyan		0.06 - 0.17
Green		0.17 - 0.28
GreenBlue		0.28 - 0.39
Blue	infinity	0.39 - 0.50

Tag name: **delay**

Description: Sets the delay of script execution for the specified number of seconds. Examples of valid arguments are 10, 1.5, .75, 20.5 If the number of seconds is not specified, then the script execution continues after 1 second

Syntax: delay {number}

number - Number of seconds

See also: set delay

Tag name: **interrupt**

Description: Interrupts the current script animation. Use the interrupt command at the top of your script to stop or change a currently executing movie (a script animation that loops)

Syntax: interrupt

See also: pause, unpause

Tag name: label residue

Description: Specifies whether to label selected residues

Syntax: label residue {true|false} or label residue (same as label residue true)

true - label the selected residues.

false - (default) do not label the selected residues.

Tag name: list

Description: Sets list visibility

Syntax: list {listname} {true|false}

true - (default) make the list visible.

false - make the list invisible.

Tag name: list color

Description: Sets the list color. This is identical to the "color list {listname} colors" command; see **color list** for details

Syntax: list {listname} color

Tag name: list transparent

Description: Sets the list transparency value

Syntax: list {listname} transparent {true|false}

true - make the list transparent.

false - (default) make the list opaque.

Tag name: list zap|delete

Description: Deletes the specified list

Syntax:

```
list {listname} zap  
list {listname} delete
```

The * character can be used as a simple wildcard. For example, "list * delete" deletes all lists; "list amino* delete" deletes all lists whose name starts with "amino".

Tag name: load {URL}

Description: Opens and loads a file. You can specify a complete or partial URL for the source location of the file. If you specify only the filename, then the file will be searched for in the same directory on the server as the script file was retrieved from. If the server does not specify a valid MIME type for the file, then the format specified by the format option will be used. Only a single molecule may be loaded at a time. To delete a molecule prior to loading another molecule, use the RasMol zap command.

Syntax: load [format] {URL}

format - valid molecule file formats are pdb, csm, csml, cub, cube, gau, emb, embl, jdx, dx, mdl, rxn, skc, tgf, xyz, mop, scr, and spt. If no file format is specified, pdb is the default.

URL- URL of the file to be loaded. URL must have less than or equal to 80 characters. Examples of valid URLs:

mymol.pdb ../mymol.pdb

http://www.source.com/location/mymol.pdb

file:///c:/folder/mymol.pdb (for Windows)

file:///Macintosh HD/folder/filename.pdb (for the Mac)

Tag name: load pmesh

Description: Loads a pmesh file, creating a surface

Syntax: load pmesh {filename} [listname]

The optional **listname** can be used in subsequent commands to refer to the surface created by this command.

Tag name: load surface gaussian

Description: Loads a Gaussian file, creating a surface

Syntax: load surface gaussian {filename} [listname]

The optional **listname** can be used in subsequent commands to refer to the surface created by this command.

Tag name: loop

Description: Causes the script execution to restart after the specified number of seconds. If a number is not specified, the default delay before looping is 1 second.

Syntax: loop {number}

number - number of seconds to wait before restarting the script

Tag name: move

Description: Starts a move animation for the specified time using relative values for various view parameters. Chime animates the structure in steps over TotalTime to reach the targets implied by the relative arguments. All arguments are numerical values. Except for FPS and MaxAccel, all arguments are required.

Syntax:

**move Xrot Yrot ZRot Zoom XTrans YTrans ZTrans Slab TotalTime [FPS]
[MaxAccel]**

XRot - Rotation integer value states the angle in degrees for the structure to be rotated. A positive value moves the closest point up and right, and a negative value moves the closest point down and left.

YRot - Rotation integer value states the angle in degrees for the structure to be rotated. A positive value moves the closest point up and right, and a negative value moves the closest point down and left.

ZRot - Rotation integer value states the angle in degrees for the structure to be rotated. A positive value rotates clockwise, and a negative value rotates anti-clockwise.

Zoom - Changes the magnification of the currently displayed image. The minimum parameter value is 1, the maximum parameter value is dependent upon the size of the molecule being displayed.

XTrans - Displacement values must be between -100 and 100. A positive value moves the molecule to the right, and a negative value moves the molecule to the left.

YTrans - Displacement values must be between -100 and 100. A positive value moves the molecule down the screen, and a negative value moves the molecule up the screen.

ZTrans - Displacement values must be between -100 and 100. The displacement rotates the molecule.

Slab - Values range from 0 at the very back of the molecule to 100 which is completely in front of the molecule. Intermediate values determine the percentage of the molecule to be drawn.

TotalTime - The 'target' total time for the entire animation in seconds.

FPS - (optional) The 'target' frames per second for the animation. The default is set to 30. On slower computers Chime will attempt to accelerate the movement in order to keep up with the target times.

MaxAccel - (optional) The maximum rate that you will allow the move to be accelerated on slow machines. $\text{MaxAccel} = \text{target frames per second (FPS)} / \text{actual frames per second}$. The default rate is set to 5. See the following notes for further information.

Notes

- Actual time will never be less than total time.
- Actual time will exceed total time only when ($\text{accel} > \text{MaxAccel}$) is needed.
- Actual FPS (aFPS) will never exceed target FPS (tFPS).
- aFPS can be less than tFPS up to $\text{tFPS/aFPS} = \text{MaxAccel}$. Acceleration is an integral divisor for tFPS. Thus, the if $\text{MaxAccel} = 5$ and $\text{tFPS} = 30$, the largest jumps possible would be $30/5 = 6 = \text{max aFPS}$.
- The acceleration occurs at more than one point during the move. Thus the first few frames can be at 30 FPS (hence small rotations), then it can drop to 15 FPS (twice as much rotation per frame, $\text{accel} = 2$), then to 10 FPS ($\text{accel} = 3$), then to 7 FPS ($\text{accel} = 4$), then to 6 FPS ($\text{accel} = 5$), but no lower if $\text{MaxAccel} = 5$.

See also: set move

Tag name: pause

Description: Temporarily stops the current script animation, until you execute the unpause command. Use button(s) that execute the pause and unpause commands to temporarily pause a movie (a script animation that loops).

Syntax: pause

See also: interrupt, unpause

Tag name: script {URL}

Description: Opens and executes a script file. You can specify a complete or partial URL for the source location of the script file. If only the filename is specified then the script file will be searched for in the same directory on the server as the script file was retrieved from. The server does NOT have to specify the 'application/x-spt' MIME type for the script file.

Syntax: script {URL}

URL - URL of the file to be executed. Examples of valid URLs:

```
myscript.spt ../myscript.scr http://www.source.com/location/dna1.top
```

Tag name: sculpt

Description: Sends a command to Sculpt to be processed by that program

Syntax: sculpt {command} or send sculpt {command}

Everything after sculpt is sent for Sculpt to interpret.

Tag name: set charge

Description: Sets the specified charge on all selected atoms. Use this to specify your own charge/other data, so that the MEP functions can map these values onto a texture mapped surface.

Syntax: set charge {charge value}

Tag name: set charge function

Description: Sets the specific charge calculation function to use for calculating charges for molecules which do not have charge information present.

Syntax:

```
set charge function {none|Gasteiger|Kollman|Charmm}
```

none - (default) Chime will choose the charge function based on the number of heteroatoms in the structure:

If ≥ 255 atoms and hydrogens present in a PDB, then Kollman partial charges are assigned for standard residues/atoms.

If ≥ 255 atoms and Kollman partial charges are not used and aminoacids are present, then Charmm 1.9 charges are assigned.

If ≥ 255 atoms and neither Kollman nor Charmm was used, then Gasteiger is used.

If < 255 atoms, then Gasteiger is used.

Gasteiger - uses Gasteiger's method of assigning partial charges.

Kollman - assigns Kollman partial charges to standard aminoacid and nucleic residues. This requires hydrogens to be present in the PDB file.

Charmm - assigns Charmm 1.9 charges to aminoacids only.

Tag name: **set clear color**

Description: Sets the color to use when blending a "clear" section of texture map with another color. The default color for the blending of clear is white. If you are blending between 2 colors in the texture map, and one is clear, then half (1/2) will be clear, and the remaining colors are blended between the clear color and the specified color. If there are 3 colors specified, and clear is one of them, then one third (1/3) of the texture map will be clear, and blending is done between the clear color and the specified colors. The gradation depends on the color scheme used. See `color list` for information on this command.

Syntax: `set clear color {color}`
or
`set transparent color {color}`

See also: `color list`

Tag name: **set delay**

Description: Disables or enables the delay interval for the subsequent `delay` commands in the script. The delay interval is the number of seconds for which a script execution is delayed. It is a parameter of the `delay` command.

Syntax:

`set delay {on|off}`

off - Sets the subsequent delay intervals to 0 seconds.

on - (default) Enables the delay interval that is specified for each subsequent `delay` command.

Notes

- `set delay` helps you debug or enhance a specific portion of your script. To disable all delay intervals except for a portion of the script that you want to execute at the intended speed:

1. Insert a `set delay off` command at the top of the script.
 2. Insert a `set delay on` command at the point in the script where you want to enable the delay intervals.
- Use `set delay off` with `set move off` to allow the script to run at maximum speed. If you want to test a specific set of commands in your script, you can "fast-forward" the script to the portion that you want to see at normal speed. You can remove these commands after you completed your tests.

The following example "fast-forwards" to a particular command, *command2*, in the script:

```
script="
set delay off
set move off
command1
move 0 0 0 0 30 0 0 0 0.5 30
move 0 0 0 0 -60 -30 0 0 0.5 30
move 0 0 0 0 30 60 0 0 0.5 30
move 0 0 0 0 0 -30 0 0 0.5 30
delay 0.3
set delay on
set move on
command2
delay 0.3
move 0 0 0 0 30 0 0 0 0.5 30
move 0 0 0 0 -60 -30 0 0 0.5 30
move 0 0 0 0 30 60 0 0 0.5 30
move 0 0 0 0 0 -30 0 0 0.5 30
more-commands
"
```

See also: `delay`, `move`, `set move`

Tag name: `set gaussian contour`

Description: Sets the contour level used when reading gaussian data files. The default contour level is 0.2 A.

Syntax: `set gaussian contour {value}`

value - real value in Angstroms.

Tag name: `set load check`

Description: By default, Chime / Chime Pro 2.0 will not execute a load command if the same molecule is being re-loaded. By calling "`set load check false`", you can override this feature, allowing the molecule to be re-loaded. This also has an effect on the `list zap` command. When `load check` is set to `true` (the default), `list zap` will be ignored because an implicit zap is done when loading a new molecule.

Syntax: `set load check {true|false}`

Tag name: `set mep mode`

Description: Set the range for MEP texture mapping

Syntax: `set mep mode {1|2|3 or rasmol}`

mode 1 - surface is colored relative to extremes of molecule.

mode 2 - (-0.10) to +0.10 range for charges

mode 3 - (-0.24) to +0.24 range for charges (what rasmol uses)

Tag name: `set mep|mlp distance`

Description: Sets the maximum distance to be considered for MEP or MLP influence calculations. The default is 8.0 angstroms

Syntax: `set {mep|potential} [distance] [within] #angstroms#`
 or
`set mlp [distance] [within] #angstroms#`

Use the keywords **mep** and **potential** interchangeably in this command.

Either **distance** or **within** is required, but not both.

Tag name: `set mep|mlp function`

Description: Specifies the function used to determine MEP or MLP distance when rendering a surface. This command is often used in conjunction with "set mep|mlp distance" to establish a distance "cutoff".

Syntax:

```
set mep function {1 or Gaillard|2 or Audry|3 or Fauchere|4 or Hartshorn|5
or Coulomb}
or
set mlp function {1 or Gaillard|2 or Audry|3 or Fauchere|4 or Hartshorn}
```

Some of the calculations used:

Function	Description
Gaillard or 1	$MLP = \sum (f * e^{(-d/2)})^{1-natoms}$ f = Lipophilic value for atom i d = distance from point to atom (angstroms) Gaillard, P., Carrupt, P.A., Testa, B. and Boudon, A., J.Comput.Aided Mol.Des. 8, 83-96 (1994)
Audry or 2	$MLP = \sum (f/(1 + d))^{1-natoms}$ f = Lipophilic value for atom i d = distance from point to atom (angstroms) Audry, E.; Dubost, J. P.; Colleter, J. C.; Dallet, P. A new approach to structure-activity relations: the "molecular lipophilicity potential". Eur. J. Med. Chem. 1986, 21, 71-72.

Fauchere or 3	MLP = Sum(f * e^{-d})/1-natoms f = Lipophilic value for atom i d = distance from point to atom (angstroms) Fauchere, J. L.; Quarendon, P.; Kaetterer, L. Estimating and representing hydrophobicity potential. J. Mol. Graphics 1988, 6, 203-206.
Hartshorn or 4	Mike Hartshorn's weighted distance algorithm
Coulomb or 5	Coulomb's law distance function (same as rasmol potential distance function)

Tag name: set mlp mode

Description: Sets the mode for mlp texture map calculations to either "absolute" or "relative"

Syntax: set mlp mode {true|false}

true - absolute scale, for comparing different molecules.

false - (default) relative scale, highest/lowest is relevant to the current molecule only.

Tag name: set move

Description: Disables or enables the animation time for the subsequent move commands in the script. The animation time is the 'target' total time for the entire animation in seconds. It is a required parameter for the move command.

Syntax:

set move {on|off}

off - Sets the animation time to 0 seconds for each subsequent move command.

on - (default) Enables the animation time that is specified as the TotalTime parameter for each subsequent movecommand.

Notes

- set move helps you debug or enhance a specific portion of your script. To disable all animation intervals except for the portion of the script that you want to execute at the intended speed:
 1. Insert a set move off command at the top of the script.
 2. Insert a set move on command at the point in the script where you want to enable the animation intervals.
- Use set move off with set delay off to allow the script to run at maximum speed. If you want to test a specific set of commands in your script, you can "fast-forward" the script to the portion that you want to see at normal speed. You can remove these commands after you completed your tests.

The following example "fast-forwards" to a particular command, *command2*, in the script:

```
script="
set delay off
set move off
command1
move 0 0 0 0 30 0 0 0 0.5 30
move 0 0 0 0 -60 -30 0 0 0.5 30
move 0 0 0 0 30 60 0 0 0.5 30
move 0 0 0 0 0 -30 0 0 0.5 30
delay 0.3
set delay on
set move on
command2
delay 0.3
move 0 0 0 0 30 0 0 0 0.5 30
move 0 0 0 0 -60 -30 0 0 0.5 30
move 0 0 0 0 30 60 0 0 0.5 30
move 0 0 0 0 0 -30 0 0 0.5 30
more-commands
"
```

See also: delay, move, set delay

Tag name: **set picking select**

Description: Allows the user to select and deselect objects using the mouse. If objects are already selected beforehand, that selection can be added to or modified by the user.

Only one type of object can be selected at a time, depending on the qualifier used in the command.

Syntax:

```
set picking select {atom|bond|chain|residue}
or
set picking select (same as set picking select atom)
```

Tag name: **set spin fps**

Description: Sets the spin frames per second. This is equivalent to the `spinfps embed` tag

Syntax: `set spin fps ###`

Tag name: **set spin x|y|z**

Description: Sets the speed of spin along the x, y, or z axis, in degrees per second. This is equivalent to the `spinX`, `spinY`, and `spinZ` embed tags.

Syntax: `set spin {x|y|z} ###`

Tag name: **set zoom center**

Description: Specifies whether to use automatic centering of the 'translation center' or 'center of rotation' while zooming.

Syntax: `set zoom center {true|false}`

true - (default) automatic centering

false - do not perform automatic centering

See Also: `translate center`

Tag name: `show atom|residue|chain|model`

Description: Show objects of the specified type

Syntax: `show {atom|residue|chain|model} [all] [identify]`

If the **all** qualifier is present, all objects of the specified type are shown. Otherwise, only the selected objects of that type are shown. If the **identify** qualifier is present, then each atom/chain name is shown as well.

Tag name: `show list`

Description: Lists the names of all display lists. If used with the optional **all** qualifier, also gives complete information about the display lists, including types and numbers of objects in the lists.

Syntax: `show list [all]`

Tag name: `show mlp`

Description: Shows MLP totals, and sum of +/- contributions, based on either SURFACE values, or VDW dots values, depending on what was used with the last MEP coloring command.

Syntax: `show mlp`

Tag name: `show pdbheader`

Description: Return a string that contains the header information in a PDB file. Multiple lines within the string are separated by the form feed character "\f"

Syntax: `show pdbheader`

Note: You can parse the returned string to format the header information. For example, you can write a JavaScript function to replace the form feed delimiter characters with line feed characters. In the following sample code, the embed tag MessageCallback is used to call the `stringReplace` function that replaces form feed characters in the PDB header string.

```
<script language='JavaScript'>
var LF = "\n";
var FF = "\f";
function stringReplace(originalString, findText, replaceText) {
    var pos = 0;
    var len = findText.length;
    pos = originalString.indexOf(findText);
    while (pos != -1) {
```

```

        preString = originalString.substring(0,pos);
        postString = originalString.substring(pos+len,originalString.length);
        originalString = preString + replaceText + postString;
        pos = originalString.indexOf(findText);
    }
    return originalString;
}

function MyMessageCallback( buttonname, message )
{
    // add this message to our message textarea....
    document.theform.chimemessages.value += stringReplace(message, FF, LF) + "\r\n";
}

</script>

<form name="theform">
<table border cellpadding=10 cellspacing=0>
<tr>
<td rowspan=2 align=center valign=middle bgcolor=black><embed width=300 height=250 sr
name="theChimePlugin" MessageCallback="MyMessageCallback"
script="select protein
        wireframe 40
        select not protein
        spacefill 250
        select water
        spacefill 0"
        extra="load pmesh surface/test.tmesh" spiny=80>
</td>
</tr>
<tr>
<td>
        <center><font size=-1>Example Command Entry Window</font></center>

        <textarea name="rasmolscript" rows=5 cols=45>
        show pdbheader
        </textarea>

        <center>
        <input type="button" onClick="document.theChimePlugin.executeScript(this.form
            name="sendbut" value="Send To Chime">
        </center>
</td>
</tr>
<tr>
<td colspan=2>
        <center><font size=-1>Chime / Chime Pro Message Output</font></center>
        <center><textarea name="chimemessages" rows=6 cols=80></textarea></center>
</td>
</tr>
</table>
</form>

```

Tag name: **show selected**

Description: Turns on/off the "highlight selection" feature, in which all of the selected objects are colored gold.

Syntax:

```
show selected {true|false}
```

or

```
show selected (same as show selected true )
```

Tag name: **show spin**

Description: Reports "spin on" or "spin off" via the MessageCallBack EMBED tag option.

Syntax: **show spin**

Tag name: **slab +|-**

Description: Allows you to use the RasMol slab command with a relative change in the slab value.

The RasMol slab command enables, disables, or positions the z-clipping plane of the molecule. The program only draws those portions of the molecule that are further from the viewer than the slabbing plane. Values range from 0 at the very back of the molecule to 100, which is completely in front of the molecule. Intermediate values determine the percentage of the molecule to be drawn.

Chime allows you to place a '+' or a '-' in front of the slab value to specify a RELATIVE change in the slab value. For example, slab +5 will add 5 to the current slab value.

Syntax:

```
slab +{value}
```

```
slab -{value}
```

value - relative change in the slab value

Tag name: **spin save|restore**

Description: Used to save the current spin state, then restore it at a later time.

Syntax: **spin {save|restore}**

Tag name: **spin true|false**

Description: Turns spin on and off

Syntax:

```
spin {true|false}
```

or

```
spin (same as spin true)
```

Tag name: **surface**

Description: Creates a surface with specified properties

Syntax:

surface [name] [color] [spacing] [probe radius] [surface smoothing
true|false]

name - name assigned to the surface for use in subsequent script commands.

color - initial color given to the surface.

spacing - ... The default spacing depends on the number of atoms in the file:

Atoms	Default Spacing
<=255	0.3 A
256-499	0.55 A
500-749	0.65 A
750-999	0.75 A
1000+	0.80 A

probe radius - The default is 1.4 A.

Tag name: **translate center**

Description: Translates the center of rotation, as specified by `center` or `set picking center` Rasmol commands, to the center of the screen. The RasMol `translate` command moves the position of the center of the molecule on the screen. Chime adds the additional `center` arguments.

Syntax:

translate center

or

translate center center

translate center all

translate center {expression}

center - Translates the 'center of rotation' (as specified by `center` or `set picking center` commands) to the center of the screen.

all - Specifies a 'translation center' to be the center of the molecule. The center of the molecule will be translated to the center of the screen.

expression - Specifies a set of atoms which will be defined as the new 'translation center'. The center of the specified atoms will be translated to the center of the screen. Refer to the Rasmol manual for a detailed description of acceptable atom expressions.

See Also `set zoom center` - for information about forcing the center of translation (or center of rotation, if no center of translation is specified) to be translated to the center of the screen after any zooming operations.

Tag name: **unpause**

Description: Resumes the current script animation that the `pause` command temporarily stopped. Use button(s) that execute the `pause` and `unpause` commands to temporarily pause a movie (a script animation that loops).

Syntax: `unpause`

See also: `interrupt`, `pause`

Tag name: **view**

Description: Specifies whether to save or restore specified views of the molecule. The orientation, translation, zoom, slabbing and center of rotation are saved or restored.

Syntax:

`view save {0-15}`

`view restore {0-15}`

`view show`

or

`view show view`

`view show user`

`view set XRot YRot ZRot Zoom XTrans YTrans ZTrans Slab CenX CenY CenZ`

save {0-15} - allows you to save the current view into one of 16 slots, numbers 0 through 15. If the slot number is omitted, it is assumed to be 0.

restore {0-15} - allows you to restore a view saved with a 'view save...' command. Again, if the slot number is omitted, it is assumed to be 0. If you restore from a slot that has not had a view saved to it, the result is a 'reset'.

show or

show view - Chime outputs a 'view set' command that can be used directly to restore the current view using the `view set ...` command.

show user - Chime outputs a list of rasmol commands that can be used to restore the current view. The result is the same as the equivalent 'view set' command, but more commands are required using standard RasMol commands.

set XRot YRot ZRot Zoom XTrans YTrans ZTrans Slab CenX CenY CenZ - this command is intended to be generated by a `view show` command. Rotations are applied in the order Z, Y, and then X.

XRot - Rotation integer value states the angle in degrees for the structure to be rotated. A positive

value moves the closest point up and right, and a negative value moves the closest point down and left.

YRot - Rotation integer value states the angle in degrees for the structure to be rotated. A positive value moves the closest point up and right, and a negative value moves the closest point down and left.

ZRot - Rotation integer value states the angle in degrees for the structure to be rotated. A positive value rotates clockwise, and a negative value rotates anti-clockwise.

Zoom - Changes the magnification of the currently displayed image. The minimum parameter value is 1, the maximum parameter value is dependent upon the size of the molecule being displayed.

XTrans - Displacement values must be between -100 and 100. A positive value moves the molecule to the right, and a negative value moves the molecule to the left.

YTrans - Displacement values must be between -100 and 100. A positive value moves the molecule down the screen, and a negative value moves the molecule up the screen.

ZTrans - Displacement values must be between -100 and 100. The displacement rotates the molecule.

Slab - Values range from 0 at the very back of the molecule to 100 which is completely in front of the molecule. Intermediate values determine the percentage of the molecule to be drawn.

CentX - Defines the point of rotation in the x plane. A value of 0 resets the center of rotation to be the center of gravity of the molecule.

CentY - Defines the point of rotation in the y plane. A value of 0 resets the center of rotation to be the center of gravity of the molecule.

CentZ - Defines the point of rotation in the z plane. A value of 0 resets the center of rotation to be the center of gravity of the molecule.

Tag name: **zap true**

Description: Allows deletion ("**zap**") of a list, even when in "**set load check true**" mode where **list zap** is normally ignored.

Syntax: **zap true**
