jV Manual

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The program 'jV' has been developed by Kengo Kinoshita (The Institute of Medical Science, The University of Tokyo) and Haruki Nakamura (Institute for Protein Research, Osaka Univeristy), as one of the activities of Protein Data Bank Japan (PDBj), supported by grant-in-aid from Institute for Bioinformatics Research and Development, Japan Science and Technology Corporation (BIRD-JST).

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1. Introduction

jV is an interactive 3D viewer program to visualize protein and nucleic acid molecules. The program reads in a PDBML file that is an XML format for PDB. Usual PDB format files are also accepted. More than one molecule files can be opened and displayed at the same time and their display models and transforms can be operated separately. In addition to molecule files, a polygon file written in XML can be read and displayed. More than one polygon files can be opened at the same time and superposed on molecule images. The XML schema of the polygon file is available. jV can perform an animation of molecules. The animation file is a PDB format file in which each frame is separated by a MODEL line.

jV runs on Java Runtime Environment (JRE) and can be used both as a standalone program and an applet. The 3D rendering is performed with the use of JOGL API. The version requirements are as follows.

- JRE (includes Java Plug-in) 1.4.2 or later (recommend 1.4.2_12)
- JOGL 1.1.1 or JSR-231

Here, Java Plug-in is required in order to use the program as an applet.

The program allows an interactive mouse control and command execution. The commnad syntax follows that of Rasmol with some modifications. In order to handle the transform of each molecule and polygon separately, every files are set to be either selected or not selected. The transform operation commands, such as rotate or translate, act only on selected files. On the other hand, every atoms in a molecule are also set to be either selected or not selected independently of whether the molecule itself is selected or not selected. Only selected atoms are the target of display model operations, such as wireframe or spacefill commands, and coloring operations.

Release note

Changes and improvements have been made as follows.

- version 3.1

    - The following commands have been added; 'animrange', 'set adjustview', 'show godata', and 'show xps3'.
    - The xPSSS expression has been added in order to select a group of atoms.
    - Several public methods have been added to the applet so as to append molecule or polygon files after the applet started.
    - The applet can send information about mouse-picked atoms to JavaScript.
- version 3.1.1
    - Some problems in GUI menu [Options]-[Hetero Atoms] and [Hydrogens] have been fixed.
    - Some problems in 'trace' command have been fixed.
- version 3.1.2
    - eF-site ID has been changed to a new format.
- version 3.1.3
    - Some problems in xps3 atom selection have been fixed.
- version 3.1.4
    - Some problems in finalization process of openGL rendering have been fixed.
- version 3.1.5
    - The output of 'show xps3' command has been modified.
    - Some problems in 'save png/jpeg' command have been fixed.
- version 3.1.6
    - Some problems in loading an empty polygon file have been fixed.
- version 3.1.7
    - Some problems in initialization process of the applet have been fixed.
- version 3.2
    - 'show site' command has been added.
- version 3.3 beta 1
    - Availabe JOGL version is restricted to JSR-231 beta 5 only.
- version 3.3
    - Both the previous JOGL (version 1.1.1) and JSR-231 are available.
    - The following commands have been added; 'set viewpoint', 'show viewpoint', 'set imagesize', and 'show imagesize'.

2. Command List

Command usage of jV follows that of Rasmol with some modifications. In the following part, command arguments that can take an arbitrary value are denoted as <value> for example, arguments restricted to several possible values are listed with / as a delimiter, and arguments that can be omitted are put in brackets {}.

2.1. anim

anim forward {<value>}
Starts animation forward. If the <value> is given, just move frames forward by the specified amount.

anim backward {<value>}
Starts animation backward. If the <value> is given, just move frames backward by the specified amount.

anim stop
Stops animation.

2.2. animframe

animframe <frame> {<file_ID>}
Sets the frame of all animation files for the specified value. When <file_ID> is given, only the specified file is processed.

2.3. animmode

animmode once
Sets the behavior of animation for 'once'. When the frame reaches the last one, animation is stopped.

animmode loop
Sets the behavior of animation for 'loop'. When the frame reaches the last one, animation is reset to the first frame and continues playing.

animmode swing
Sets the behavior of animation for 'swing'. When the frame reaches the last one, the direction of animation is reversed.

2.4. animrange

animrange <init_frame>-<term_frame> {<file_IDs>}
Sets the range of all animation files. When is given, only the specified file is processed.

2.5. animselect

animselect {-a/-r} <file_IDs>
Selects the specified files and makes the others not selected. More than one file IDs can be specified

by putting commas as the delimiter. When the option -a or -r is specified, only the selection status of the specified files are modified, selected or not selected, respectively, and the others remain unchanged.

2.6. animspeed

`animspeed <speed>`
Sets the animation speed. The argument should be an integer value from 1 to 20.

2.7. animstep

`animstep <step> {<file_ID>}`
Sets the step of all animation files for the specified value. When <file_ID> is given, only the specified file is processed.

2.8. backbone

`backbone {on/true}`
Turns on the selected backbone bonds.

`backbone off/false`
Turns off the selected backbone bonds.

`backbone <radius>`
Turns on the selected backbone bonds with the specified raidus (angstrom or Rasmol unit). The maximum parameter value is 2.0.

2.9. background

`background <color>`
Changes the background color. The color may be given as RGB values [r,g,b], or predefined color names.

2.10. cartoon

`cartoon {on/true}`
Turns on the thick ribbons for the selected residues.

`cartoon off/false`
Turns off the thick ribbons for the selected residues.

`cartoon <half_width>`
Turns on the thick ribbons for the selected residues with the specified half width (angstrom or Rasmol unit). The maximum parameter value is 4.0.

2.11. center

center {-r/-s} {<atom_expression>}
Sets the center of rotation and the center of the screen to the center of a group of atoms specified by the atom expression. When the option -r or -s is specified, only the center of rotation or the center of the screen is modified, respectively.

center {-r} [x, y, z]
Moves the center of rotation and the center of the screen from the current position by the specified amount. When the option -r is specified, only the center of rotation is modified.

center {-r} {x, y, z}
Sets the center of rotation and the center of the screen to the specified coordinates. When the option -r is specified, only the center of rotation is modified.

center -s [x, y]
Moves the center of the screen from the current position by the specified amount.

center -s {x, y}
Sets the center of the screen to the specified coordinates.

2.12. color

color {atoms} <color>
Sets the color of the selected atoms. The color may be given as RGB values [r,g,b], predefined color names, or predefined color schemes; amino, chain, charge, cpk, group, shapely, structure, and temperature.

color bonds/backbone/ribbons/hbonds/ssbonds <color>
Sets the color of the specified object. The color may be given as RGB values [r,g,b] or predefined color names. For hydrogen bonds, color scheme 'type' can be specified.

color bonds/backbone/ribbons/hbonds/ssbonds none
Resets the color of the specified object.

2.13. colorvertex

colorvertex <color>
Sets the color of the selected vertices. The color may be given as RGB values [r,g,b] or predefined color names.

colorvertex none
Resets the color of the selected vertices.

2.14. cpk

cpk
A synonym of the spacefill command.

2.15. define

define <name> <atom_expression>
Associates an arbitrary set of atoms with a unique name.

2.16. display

display all
Displays the image of all files.

display none
Turns off the image of all files.

display {-a/-r} <file_IDs>
Displays the image of the specified files and turns off the others. More than one file IDs can be specified by putting commas as the delimiter. When the option -a or -r is specified, turns the image of the specified files on or off, respectively, and the others remain unchanged.

2.17. displayvertex

displayvertex {on/true}
Displays the selected vertices.

displayvertex off/false
Turns off the selected vertices.

2.18. echo

echo <string>
Echoes the specified message back to the message area.

2.19. exit

exit
Terminates the application.

2.20. fit

fit <file1_ID> <file2_ID>
Sets the transform matrix of file1 identical to that of file2.

2.21. fselect

fselect all
Selects all files.

fselect none
Selects no files.

fselect {-a/-r} <file_IDs>
Selects the specified files and makes the others not selected. More than one file IDs can be specified by putting commas as the delimiter. When the option -a or -r is specified, only the selection status of the specified files are modified, selected or not selected, respectively, and the others remain unchanged.

2.22. hbonds

hbonds {on/true}
Turns on the selected hydrogen bonds.

hbonds off/false
Turns off the selected hydrogen bonds.

hbonds <radius>
Turns on the selected hydrogen bonds with the specified raidus (angstrom or Rasmol unit). The maximum parameter value is 2.0.

2.23. load

load {pdbml} <filename> {fit <file_ID>}
Opens a PDBML file. URL can be used to open a remote file. On loading, the transform matrix can be set identical to that of the specified file.

load pdb <filename> {fit <file_ID>}
Opens a PDB file. URL can be used to open a remote file. On loading, the transform matrix can be set identical to that of the specified file.

load polygon <filename> {fit <file_ID>}
Opens a polygon file. URL can be used to open a remote file. On loading, the transform matrix can be set identical to that of the specified file.

load animation <filename> {fit <file_ID>}
Opens an animation file. URL can be used to open a remote file. On loading, the transform matrix can be set identical to that of the specified file.

load ftp <PDB_code> {fit <file_ID>}
Retrieves a PDBML file from the PDBj FTP site and opens it. On loading, the transform matrix can be set identical to that of the specified file.

2.24. pause

pause
Stops the execution of a script file until any key is pressed to restart.

2.25. quit

quit

A synonym of the exit command.

2.26. refresh

refresh
Redraws all images.

2.27 reset

2.27.1 default

reset
Restores the original viewing transformation of all images, the center of rotation, and the view point.

2.27.2 cartoon

reset cartoon
Restores the thickness of the cartoon representation.

2.27.3 line_width

reset line_width
Restores the width of lines in polygon images.

2.27.4 pickradius

reset pickradius
Restores the mouse-pickable region of each atom.

2.27.5 point_size

reset point_size
Restores the size of points in polygon images.

2.27.6 polyline_width

reset polyline_width
Restores the width of polylines in polygon images.

2.27.7 transparency

reset transparency
Restores the transparency of polygon images.

reset point_transparency
Restores the transparency of points in polygon images.

reset line_transparency
Restores the transparency of lines in polygon images.

reset triangle_transparency

Restores the transparency of triangles in polygon images.

reset quad_transparency
Restores the transparency of quads in polygon images.

reset polyline_transparency
Restores the transparency of polylines in polygon images.

2.28. ribbons

ribbons {on/true}
Turns on the ribbon surfaces for the selected residues.

ribbons off/false
Turns off the ribbon surfaces for the selected residues.

ribbons <half_width>
Turns on the ribbon surfaces for the selected residues with the specified half width (angstrom or Rasmol unit). The maximum parameter value is 4.0.

2.29. rotate

rotate x/y/z <angle>
Rotates images about the specified axis by the specified angle in degrees.

2.30. save

save {pdb} <filename>
Saves the currently selected set of atoms in a PDB format file.

save script <filename>
Creates a script file that reproduces the currently displayed image.

save png <filename>
Creates a PNG image file of the currently displayed image.

save jpeg <filename> {<quality>}
Creates a JPEG image file of the currently displayed image. The compression quality can be specified, 0 < quality <= 1, where 'quality = 1' means no compression.

2.31 script

script <filename>
Opens and executes the specified script file. URL can be used to open a remote file.

2.32 select

select
Selects all atoms. Whether hetero atoms and hydrogens are selected or not depends on the internal parameters, hetero and hydrogen, respectively.

select all
Selects all atoms including hetero atoms and hydrogens.

select none
Selects no atoms.

select <atom_expression>
Selects a group of atoms specified by the atom expression.

2.33. selectvertex

selectvertex {all}
Selects all vertices.

selectvertex none
Selects no vertices.

selectvertex <vertex_expression>
Selects a group of vertices specified by the vertex expression.

2.34 set

2.34.1 adjustview

set adjustview on
The view point is automatically adjusted when a new file is loaded.

set adjustview off
The view point is kept unchanged when a new file is loaded.

2.34.2 background

set background <color>
Changes the background color. The color may be given as RGB values [r,g,b], or predefined color names.

2.34.3 bondmode

set bondmode and
Specifies how to select an individual bonds. A bond is selected when both atoms connected by the bond are selected.

set bondmode or
Specifies how to select an individual bonds. A bond is selected when either of the connected atoms is selected.

2.34.4 cartoon

`set cartoon {<value>}`
Specifies the thickness of the cartoon representation (angstrom or Rasmol unit). The maximum parameter value is 2.0. When the parameter is not specified, it is restored to the default value.

2.34.5 center

`set center <atom_expression>`
Sets the default center of the selected files to the center of the specified atoms.

`set center [x, y, z]`
Sets the default center of the selected files to the specified coordinates.

2.34.6 drawlevel

`set drawlevel <value>`
Specifies precision of the rendering of spheres and cylinders. The value may be given as an integer (minimum 5) that stands for the number of straight line segments to represent an arc of 180 degrees.

2.34.7 hbonds

`set hbonds backbone`
Hydrogen bonds are displayed between backbones.

`set hbonds sidechain`
Hydrogen bonds are displayed between sidechains.

2.34.8 hetero

`set hetero on`
Sets the default behavior of the select command such that hetero atoms are selected.

`set hetero off`
Sets the default behavior of the select command such that hetero atoms are not selected.

2.34.9 hydrogen

`set hydrogen on`
Sets the default behavior of the select command such that hydrogens are selected.

`set hydrogen off`
Sets the default behavior of the select command such that hydrogens are not selected.

2.34.10 imagesize

`set imagesize <width> <height>`
Sets the size of the 3D-rendering panel in pixels. The size will be set within the screen size with the width being an even integer.

2.34.11 line_width

`set line_width <value>`

Sets the width of lines in polygon images. The <value> should be larger than 0.

2.34.12 loadcenter

set loadcenter on
When a file is opened, sets the default center of that file to the center of all files that have already opened.

set loadcenter off
When a file is opened, sets the default center of that file according to its own coordiantes.

2.34.13 picking

set picking off
Turns off the mouse picking.

set picking ident
Sets the mouse picking behavior to show atom identification.

set picking coord
Sets the mouse picking behavior to show atom coordinates with identification.

set picking distance
Sets the mouse picking behavior to show the distance between atoms successively picked.

set picking center
Sets the mouse picking behavior to specify the center of rotation and center of the screen.

set picking select
Sets the mouse picking behavior to select the file that contains the atom picked.

2.34.14 pickradius

set pickradius <value>
Sets the mouse-pickable region of each atom to be the sphere centered to each atom with the specified radius (angstrom or Rasmol unit).

2.34.15 point_size

set point_size <value>
Sets the size of points in polygon images. The <value> should be larger than 0.

2.34.16 polyline_width

set polyline_width <value>
Sets the width of polylines in polygon images. The <value> should be larger than 0.

2.34.17 projection

set projection perspective
Sets the projection mode for a perspective projection.

set projection parallel {<size>}

Sets the projection mode for a parallel projection. The size of image (fit to the height of the screen) can be specified (angstrom or Rasmol unit).

2.34.18 specular

`set specular on/true`
Enables the display of specular highlights on solid objects.

`set specular off/false`
Disables the display of specular highlights on solid objects.

`set specular <value>`
Enables the display of specular highlights on solid objects. The value between 0 and 100 specifies the specular color in gray scale with 0 and 100 being black and white, respectively. The default value is 50.0.

2.34.19 specpower

`set specpower <value>`
Sets the shininess of solid objects. The value between 0 and 100 specifies a material reflection coefficient with 0 being diffuse surfaces and 100 being shiny surfaces.

2.34.20 ssbonds

`set ssbonds backbone`
Disulfide bonds are displayed between backbones.

`set ssbonds sidechain`
Disulfide bonds are displayed between sidechains.

2.34.21 stereo

`set stereo`
A synonym of the stereo command.

2.34.22 transparency

`set transparency <value>`
Sets the transparency of polygon images.

`set point_transparency <value>`
Sets the transparency of points in polygon images.

`set line_transparency <value>`
Sets the transparency of lines in polygon images.

`set triangle_transparency <value>`
Sets the transparency of triangles in polygon images.

`set quad_transparency <value>`
Sets the transparency of quads in polygon images.

`set polyline_transparency <value>`

Sets the transparency of polylines in polygon images.

2.34.23 viewpoint

`set viewpoint {x, y, z}`
Sets the viewpoint to the specified coordinates.

2.35. show

`show godata`
Displays gene ontology data of molecules.

`show imagesize`
Displays the size of the 3D-rendering panel.

`show information`
Displays a detail discription of molecules.

`show site {<prefix>:<db>:<category>}`
Displays site information in an external database.

`show transform`
Displays the transform matrix of molecules.

`show viewpoint`
Displays the current viewpoint.

`show xps3`
Displays keywords available in xps3 selection.

2.36. slab

`slab {on/true}`
Enables the z-clipping plane of molecules and polygons.

`slab off/false`
Disables the z-clipping plane of molecules and polygons.

`slab <ratio>`
Sets the position of the z-clipping plane of molecules and polygons. The parameter may be given as a number from 0 to 100. The values 0 and 100 represent that image as a whole is completely invisible and visible, respectively.

`slab -v <value>`
Sets the position of the z-clipping plane of molecules and polygons by specifying the z coordinate value.

2.37. spacefill

spacefill {on/true}
Turns on the ball image of the selected atoms.

spacefill off/false
Turns off the ball image of the selected atoms.

spacefill <radius>
Turns on the ball image of the selected atoms with the specified radius (angstrom or Rasmol unit). The maximum parameter value is 3.0.

spacefill temperature
Turns on the ball image of the selected atoms using the temperature factor as radius.

2.38. ssbonds

ssbonds {on/true}
Turns on the selected disulfide bonds.

ssbonds off/false
Turns off the selected disulfide bonds.

ssbonds <radius>
Turns on the selected disulfide bonds with the specified raidus (angstrom or Rasmol unit). The maximum parameter value is 2.0.

2.39. stereo

stereo {on/true}
Enables stereo display. This command without arguments cycles three state; 'stereo off', 'stereo on' in cross-eyed mode and 'stereo on' in parallel-eyed mode.

stereo off/false
Disables stereo display.

stereo <angle>
Enables stereo display with the specified separation angle. Positive and negative values represent cross-eyed and parallel-eyed viewing, respectively.

2.40. structure

structure
Estimates the secondary structure using Kabsch and Sander's DSSP algorithm.

2.41. trace

trace {on/true}
Turns on a tube representation for the selected residues.

`trace off/false`
Turns off a tube representation for the selected residues.

`trace <radius>`
Turns on a tube representation for the selected residues with the specified radius (angstrom or Rasmol unit). The maximum parameter value is 2.0.

2.42. translate

`translate x/y/z <value>`
Moves images along the specified axis by the specified amount (angstrom).

2.43. wireframe

`wireframe {on/true}`
Turns on the selected bonds.

`wireframe off/false`
Turns off the selected bonds.

`wireframe <radius>`
Turns on the selected bonds with the specified raidus (angstrom or Rasmol unit). The maximum parameter value is 2.0.

2.44. write

`write`
A synonym of the save command.

2.45. zap

`zap {<file_IDs>}`
Closes the specified files. More than one file IDs can be specified by putting commas as the delimiter. When the paraneter is absent, all files are closed.

2.46. zoom

`zoom {<value>}`
Sets the magnification of the image as a whole. The value stands for the magnification as a percentage of the current scale. The minimum parameter value is 10.0.

3. Atom Expression

In order to specify a group of atoms in a molecule, the following five expressions are available.

The standard boolean connectives 'and', 'or' and 'not', and brackets can be used to construct a complex expression. The boolean connectives may be abbreviated as '&', '|', and '|', respectively.

3.1. predefined set

3.1.1 element name

Element names, such as carbon or nitrogen, can be used to select atoms.

3.1.2 set based on residue property

a) amino acids in protein molecule

	ALA	ARG	ASN	ASP	CYS	GLU	GLN	GLY	HIS	ILE	LEU	LYS	MET	PHE	PRO
Acidic				*		*									
Acyclic	*	*	*	*	*	*	*	*		*	*	*	*		
Aliphatic	*							*		*	*				
Aromatic									*					*	
Basic		*							*			*			
Buried	*				*					*	*		*	*	
Charged		*		*		*			*			*			
Cyclic									*					*	*
Hydrophobic	*							*		*	*		*	*	*
Large		*				*	*		*	*	*	*	*	*	
Medium			*	*	*										*
Negative				*		*									
Neutral	*		*		*		*	*	*	*	*		*	*	*
Polar		*	*	*	*	*	*		*			*			
Positive		*							*			*			
Small	*							*							
Surface		*	*	*		*	*	*	*			*			*
Cysteine					*										
Amino	above 20 amino acids + ASX, GLX, PCA, HYP														
Protein	above 20 amino acids + ASX, GLX, PCA, HYP, UNK, ACE, FOR														

b) nucleotides

	A	C	G	T	U	+U	I	1MA	5MC	OMC	1MG	2MG	M2G	7MG	OMG	YG	H2U	5MU	PS
AT	*			*															
CG		*	*																
Purine	*		*																

Pyrimidine		*		*															
DNA	*	*	*	*															
RNA	*	*	*		*	*	*	*	*	*	*	*	*	*	*	*	*	*	*
Nucleic	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*	*

c) others

	HOH	DOD	SO4	PO4
Water	*	*		
Ions			*	*
Solvent	*	*	*	*

3.1.2 others

Alpha	atoms whose name is CA.
Hetero	atoms written as HETATM in PDB files or atoms in Solvent set.
Ligand	atoms in Hetero set and not in Solvent set.
Backbone Mainchain	atoms in Amino set whose name is N, CA, C or O, or atoms in Nuceic set whose name is P,O1P,O2P,O5*,C5*,C4*,O4*,C3*,O3*,C2*,O2* or C1*.
Sidechain	atoms in Amino set or Nucleic set and not in Backbone set.
Bonded	atoms that is connected to at least one other atom.
Selected	atoms currently selected.
Helix	atoms in the alpha-helix structure.
Sheet	atoms in the beta-sheet structure.
Turn	atoms in the turn structure.

3.2. comparison operators

Parts of a molecule can be selected using equality, inequality and ordering operators on their properties. Possible operators are =, ==, <>, !=, /=, <, <=, > and >=, and possible property names are as follows.

AtomNo	atom ID in PDB files.
ElemNo	atomic number.
ResNo	residue ID in PDB files.
Radius	radius of a ball image of atoms.
Temperature	temperature factor of atoms.
Model	model ID in PDB files.
File	File ID.

3.3. residue range

A group of atoms in a molecule can be selected by the residue ID. For example, command 'select 3' selects atoms whose residue ID is 3, and 'select 3-10' selects atoms whose residue ID is larger than or equal to 3 and smaller than or equal to 10.

3.4. within expression

A within expression selects atoms that exist within a specified distance from another set of atoms. For example, 'select within(3.0, backbone) selects atoms within a 3.0 Angstrom radius of any atom in a protein or nucleic acid backbone.

3.5. xPSSS expression

A xPSSS expression selects a group of atoms according to molecule's properties defined in the 'PDBML plus' file. It takes the following form;
  xps3:keyword.
For example, 'select xps3:binding'. The keywords available for each molecule are obtained by the 'show xps3' command.

3.6. primitive expression

A primitive expression takes such a form as
  'residue name [residue ID][:chain ID][.atom name][;alternate location][/model ID][@file ID]'.
Here, residue name and atom name are three letter and four letter name, respectively, and terms in square brackets can be omitted. For example, command 'select SER.CA' selects all alpha carbon atoms in serine.

4. Vertex Expression

In order to specify a group of vertices in a polygon, the following three expressions are available.

The standard boolean connectives 'and', 'or' and 'not', and brackets can be used to construct a complex expression. The boolean connectives may be abbreviated as '&', '|', and '|', respectively.

4.1. comparison operators

Parts of a polygon can be selected using equality and inequality operators on the ID numbers assigned to each vertex; for example, id >= 100. Possible operators are =, ==, <>, !=, /=, <, <=, > and >=. When each vertex element has a user_data element, every attributes in the user_data element can be used to select vertices with equality and inequality operators.

4.2. within expression

A within expression selects vertices that exist within a specified distance from a set of atoms.
  1) within(<distance>, <atom_expression>)
Instead of a set of atoms, a single point coordinates, from which the distance is measured, can be specified.
  2) within(<distance>, [x, y, z])
  3) within(<distance>, {x, y, z})
In case 2), vertices are selected according to their current coordinates displayed in the screen. On the other hand, coordinates written in the original polygon file are used in case 3).

4.3. box expression

A box expression selects vertices that exist in some cubes, where each cube is centered to each atom

in a specified set of atoms. The syntax is similar to that of the within expression.
1) box(<size>, <atom_expression>)
When a single point coordinates is given in the second argument, vertices that exist in a single cube, whose center is set to the passed coordinates, are selected.
2) box(<size>, [x, y, z])
3) box(<size>, {x, y, z})
In every cases, the length of an edge of the cubes is twice as the specified value.

5. Color Expression

5.1. RGB values

A color can be specified by a comma separated triple of Red, Green and Blue (RGB) components enclosed in square brackets, where RGB values are from 0 to 255, respectively.

5.2. Predefined Color

The following 24 colors can be specified by their name.

color name	RGB values	color
BLACK	[0, 0, 0]	
BLUE	[0, 0, 255]	
BLUETINT	[175, 214, 255]	
BROWN	[175, 117, 89]	
CYAN	[0, 255, 255]	
GOLD	[255, 156, 0]	
GREY	[125, 125, 125]	
GREEN	[0, 255, 0]	
GREENBLUE	[46, 139, 87]	
GreenTint	[152, 255, 179]	
HOTPINK	[255, 0, 101]	
MAGENTA	[255, 0, 255]	
ORANGE	[255, 165, 0]	

PINK	[255, 101, 117]	
PINKTINT	[255, 171, 187]	
PURPLE	[160, 32, 240]	
RED	[255, 0, 0]	
REDORANGE	[255, 69, 0]	
SEAGREEN	[0, 250, 109]	
SKYBLUE	[58, 144, 255]	
VIOLET	[238, 130, 238]	
WHITE	[255, 255, 255]	
YELLOW	[255, 255, 0]	
YELLOWTINT	[246, 246, 117]	

5.3. Color Scheme

5.3.1 amino

The color scheme 'amino' colors amino acids as follows.

amino acids	RGB values	color
ASP, GLU	[230,230, 10]	
CYS, MET	[230,230, 0]	
LYS, ARG	[20, 90,255]	
SER, THR	[250,150, 0]	
PHE, TYR	[50, 50,170]	
ASN, GLN	[0,220,220]	
GLY	[235,235,235]	
LEU, VAL, ILE	[15,130, 15]	
ALA	[200,200,200]	
TRP	[180, 90,180]	
HIS	[130,130,210]	
PRO	[220,150,130]	
Others	[190,160,110]	

5.3.2 chain

The color scheme 'chain' assigns each macromolecular chain a unique colour.

5.3.3 charge

The color scheme 'charge' colors atoms according to their temperature factor. High values are coloured in blue and lower values coloured in red.

5.3.4 cpk

The color scheme 'cpk' colors atoms according to the element type as follows.

element	RGB values	color
C	[200, 200, 200]	
N	[143, 143, 255]	
O	[240, 0, 0]	
S	[255, 200, 50]	
H	[255, 255, 255]	
He	[255, 192, 203]	
F, Si, Au	[218, 165, 32]	
Na	[0, 0, 255]	
P, Fe, Ba	[255, 165, 0]	
Al, Ca, Ti, Cr, Mn, Ag	[128, 128, 144]	
Ni, Cu, Zn, Br	[165, 42, 42]	
I	[160, 32, 240]	
B, Cl	[0, 255, 0]	
Li	[178, 34, 34]	
Mg	[34, 139, 34]	
Others	[255, 20, 147]	

5.3.5 group

The color scheme 'group' colors residues by their position in a macromolecular chain. Each chain is drawn as a smooth spectrum from blue to red. The N terminus of proteins and 5' terminus of nucleic acids are colored red and the C terminus of proteins and 3' terminus of nucleic acids are drawn in blue.

5.3.6 shapely

The color scheme 'shapely' colors residues as follows.

residue	RGB values	color
ALA	[140, 255, 140]	
GLY	[255, 255, 255]	
LEU	[69, 94, 69]	
SER	[255, 112, 66]	
VAL	[255, 140, 255]	
THR	[184, 76, 0]	
LYS	[71, 71, 184]	
ASP	[160, 0, 66]	
ILE	[0, 76, 0]	
ASN	[255, 124, 112]	
GLU	[102, 0, 0]	

PRO	[82, 82, 82]	
ARG	[0, 0, 124]	
PHE	[83, 76, 66]	
GLN	[255, 76, 76]	
TYR	[140, 112, 76]	
HIS	[112, 112, 255]	
CYS	[255, 255, 112]	
MET	[184, 160, 66]	
TRP	[79, 70, 0]	
A	[160, 160, 255]	
C	[255, 140, 75]	
G	[255, 112, 112]	
T	[160, 255, 160]	
Others	[255, 0, 255]	

5.3.7 structure

The color scheme 'structure' colors residues according to the secondary structure as follows.

secondary structure	RGB values	color
alpha helix	[255, 0, 128]	
beta sheet	[255, 200, 0]	
turn	[96, 128, 255]	
none	[255, 255, 255]	

5.3.8 temperature

The color scheme 'temperature' colors atoms according to their temperature factor. High values are coloured in red and lower values coloured in blue.

5.3.9 type

This color scheme 'type' colors each hydrogen bond according to the distance along a protein chain between hydrogen bond donor and acceptor as follows.

offset	RGB values	color
+2	[255, 255, 255]	
+3	[255, 0, 255]	
+4	[255, 0, 0]	
+5	[255, 165, 0]	
-3	[0, 255, 255]	
-4	[0, 255, 0]	
Others	[255, 255, 0]	

6. Use as Applet

6.1. Introduction

In order to use jV as an applet, Java Plug-in must be installed on client computers. The applet is called from usual APPLET tags, or OBJECT and EMBED tags in HTML (see Java Plug-in homepage), where class name that should be called is "org.pdbj.viewer.gui.ViewerApplet" class. The program has following features.

- whether to use the command line interface or not can be specified
- whether to use the file control panel or not can be specified
- whether to use the popup menu or not can be specified
- witihin applets in the same web page, mouse events can be shared
- applet can receive a command string from JaveScript
- applet can send information about mouse-picked atoms to JavaScript.

6.2. Parameters

To initialize the applet, the following parameters can be specified in HTML.

parameter	value
pdbmlURL	URL of the PDBML files to be loaded (delimited by comma for more than one files).
pdbURL	URL of the PDB files to be loaded (delimited by comma for more than one files).
polygonURL	URL of the polygon files to be loaded (delimited by comma for more than one files).
animURL	URL of the animation files to be loaded (delimited by comma for more than one files).
command_area	whether to use the command line interface or not (true or false).
file_control	whether to use the file control panel or not (true or false).
popup_menu	whether to use the popup menu or not (true or false).
mouse_send_to	name property of applets with which mouse events are shared (delimited by comma for more than one applets).
commands	initial commands that are executed when the applet starts (delimited by semicolon for more than one commands).
report_picking	whether to send information about mouse-picked atoms to JavaScript or not (true or false).

6.3. JavaScript-to-Applet Communication

The ViewerApplet class has some public methods, which can be called from JavaScript.

```
void executeCommand(String commands)
```

Through this method, the applet can receive some arbitrary commands (delimited by semicolon).

```
void loadPDB(String fileLocation)
void loadPDBML(String fileLocation)
void loadPolygon(String fileLocation)
void loadAnim(String fileLocation)
```

Using these methods, PDB file, PDBML file, polygon file, and animation file specified by URL can be loaded respectively.

```
void loadPDB(String fileLocation, int fitTo)
void loadPDBML(String fileLocation, int fitTo)
void loadPolygon(String fileLocation, int fitTo)
void loadAnim(String fileLocation, int fitTo)
```

When these methods are used, the transform matrix of the loaded file is set identical to that of the specified file.

6.4. Applet-to-JavaScript Communication

In order to send the result of mouse-picking to JavaScript, the following function must be defined in JavaScript.

```
function receiveMousePick(file, model, chain, res, atom, altloc, resName,
atomName, x, y, z)
```

In addition, a new attribute 'MAYSCRIPT' is required in APPLET or OBJECT/EMBED tags (see Java Plug-in guide).