User Manual of Web3DMol

Written by Maoxiang Shi
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Introduction

Web3DMol is an application used for displaying 3D structure of proteins on web browsers.

Input : PDB files

Output : 3D structure graphics as well as other important information

Technology

• Constructed with **HTML**, **CSS** and **JavaScript** (totally client-side technology, no server-side languages involved).

• **WebGL** is applied to Web3DMol in order to gain GPU acceleration.

• Supported by most modern browsers (Table.1).

Table 1. Requirement for web browsers to run Web3DMol

Web Browser	Support Version	Support Since
Chrome	8.0+	Dec 02, 2010
Firefox	4.0+	Mar 22, 2011
Safari	5.1+	Jul 20, 2011
Opera	12.1+	Nov 05, 2012
Internet Explorer	Edge	Jul 29, 2015
iOS Safari	8.0+	Sep 17, 2014
Opera Mobile	37+	Sep 23, 2016
Android WebView	Chromium 56+	Feb 01, 2017
Chrome for Android	57+	Mar 27, 2017

Usage

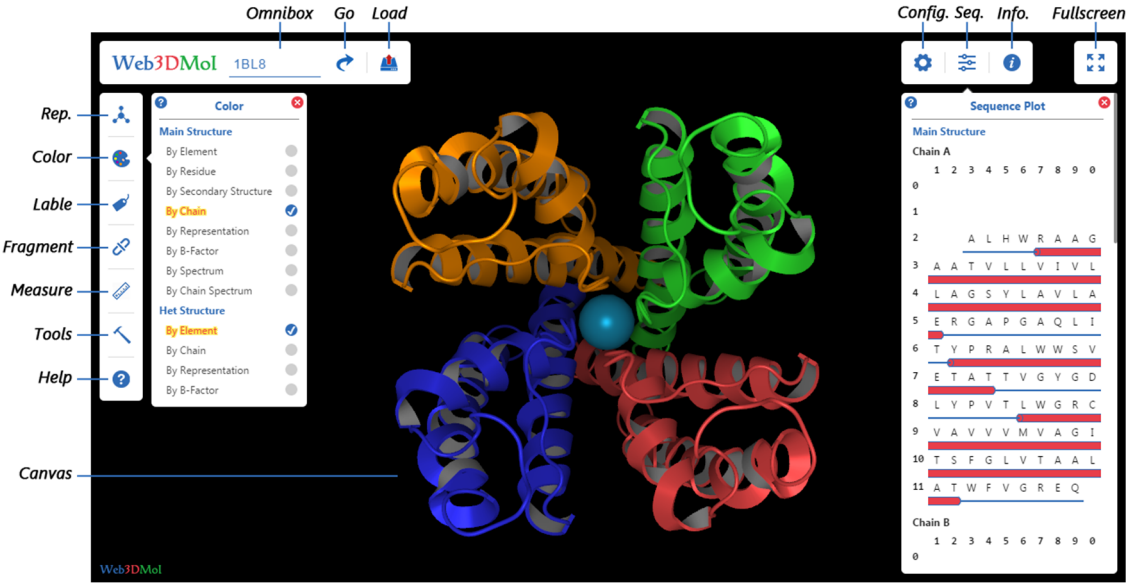


Figure 1. Common user interface of Web3DMol

Initialization

Three ways to initialize Web3DMol:

1. Visit http://web3dmol.duapp.com/;

2. Download Source Code, unzip and double-click index.html;

3. Embed Web3DMol into other applications, then initialize the application.

Load PDB

Load from RCSB

Input PDB-ID in Omnibox, then press ***ENTER*** key or click ***GO*** button.

Load from Local File System (two ways)

1. Click ***Load*** button, then select a pdb file from local file system.

2. Simply ***drag*** a pdb file from local file system and ***drop*** it into Web3DMol interface.

(NOTE : Local pdb file will NOT be uploaded.)

Interaction

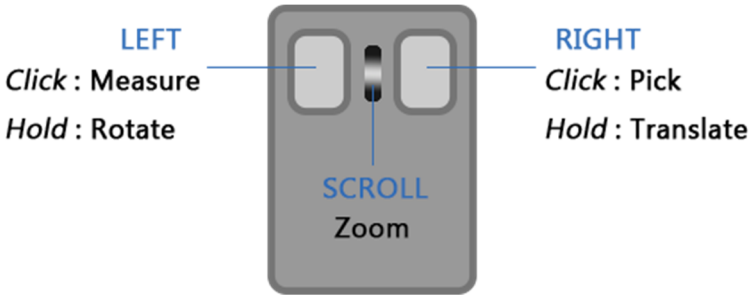


Figure 2. Function of Mouse

Rotate	Press & hold **LEFT** mouse, then move.
Translate	Press & hold **RIGHT** mouse, then move.
Zoom	Scroll **UP** to zoom in; scroll **DOWN** to zoom out.
Pick	Click **RIGHT** mouse on the 3D structure.
Measure	Click **LEFT** mouse on the 3D structure. (A measurement must be started before left-click takes effect. Also see *Measure Plane*.)

Main & Het Structure

There are two different kinds of atom recorded in PDB files.

Main ATOM

Standard amino acids and nucleotides.

Het (heterogenic) HETATM

Non-standard residues, such as prosthetic groups, inhibitors, solvent molecules and ions.

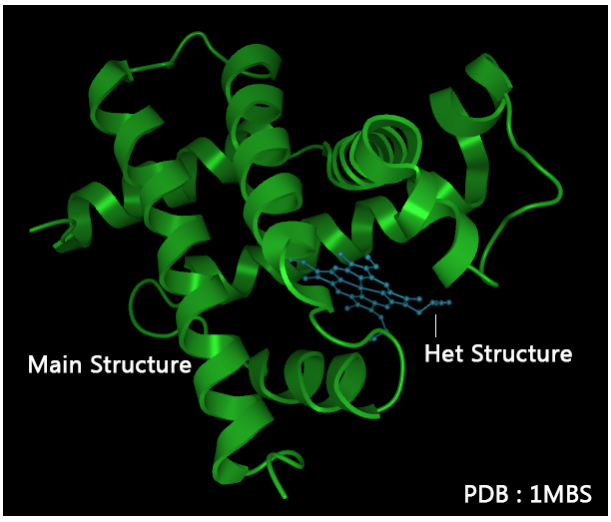


Figure 3. Main & Het structure

Representation Mode

Representation mode can be adjusted in **Representation Plane**.

Hide	Show nothing.
Dot	Atom are shown as dots.
Line	Atoms are connected by line according to residues' molecular structure.
Backbone	Atoms in the main chain are connected by tubes.
Tube	Residues are connected along the main chain by tubes.
Cartoon	Residues are connected along the main chain according to secondary structure. By default, α-helixes and β-sheets are connected by cubes, while random coils are connected by tubes.

Cartoon Variants

Cartoon-Putty	Residues are connected along the main chain by tubes. Tube's radius varies according to the B-factor.
Cartoon-Cube	Residues are connected along the main chain by cubes. The connector’s cross section is rectangle.
Cartoon-Strip	Residues are connected along the main chain. The connector’s cross section is like a playground racetrack.
Cartoon-Ribbon	Residues are connected along the main chain. The connector’s cross section is oval.
Cartoon-Railway	Residues are connected along the main chain. The connector’s cross section is like a dumbbell.
Cartoon-Cylinder	The first and last residue are connected by a straight tube. The radius of tube is much fatter than radius in Tube Mode. (NOTE : Only available for α-helix in Cartoon Mode.)
Cartoon-Arrow	Residues are connected along the main chain by cubes. The width of cube at last residue varies to make an arrowhead. (NOTE : Only available for β-sheet in Cartoon Mode.)

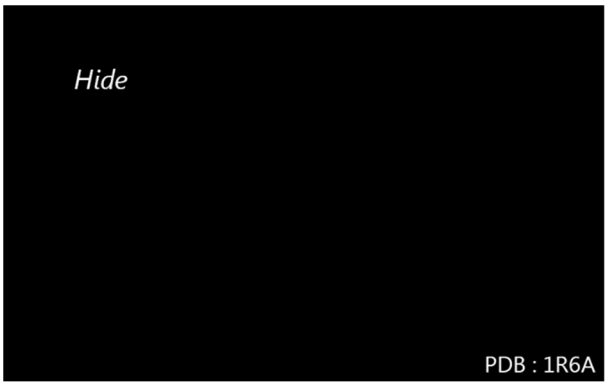
Stick Atoms are connected by tube according to residues' molecular structure.

Sphere Atoms are shown as spheres.

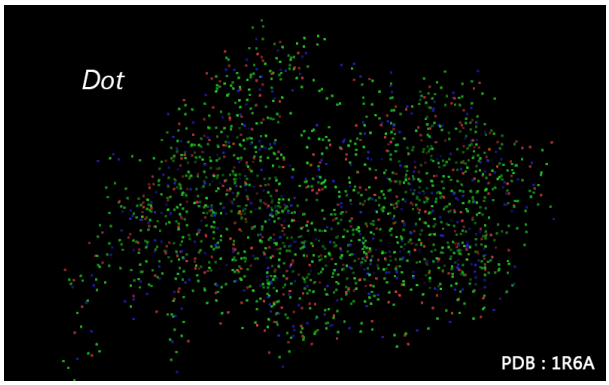
The radius of spheres varies according to atoms' van der Waals radius.

Ball & Rod Atoms are shown as spheres and connected by thin rods.

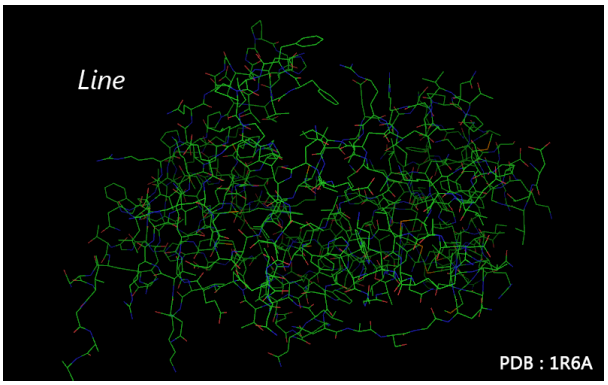
(NOTE : Only available for Het Structure or Single Residue.)



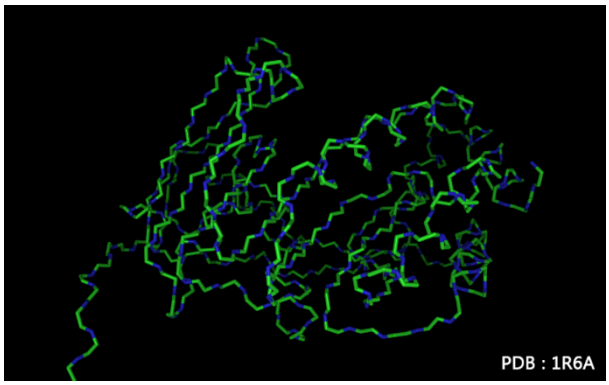
(a) Hide



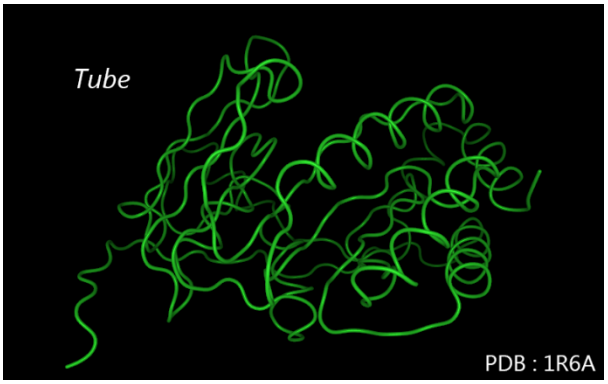
(b) Dot



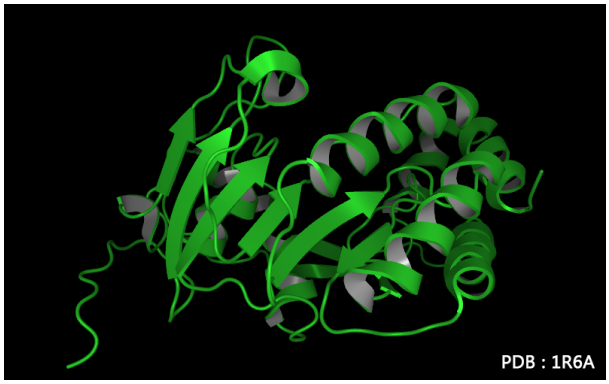
(c) Line



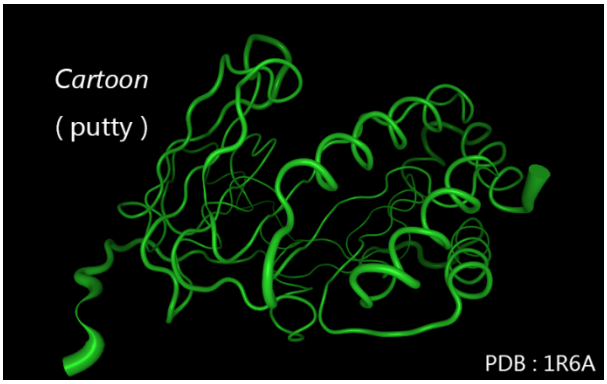
(d) Backbone



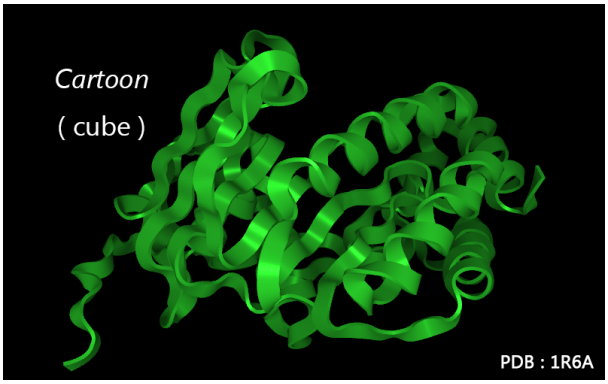
(e) Tube



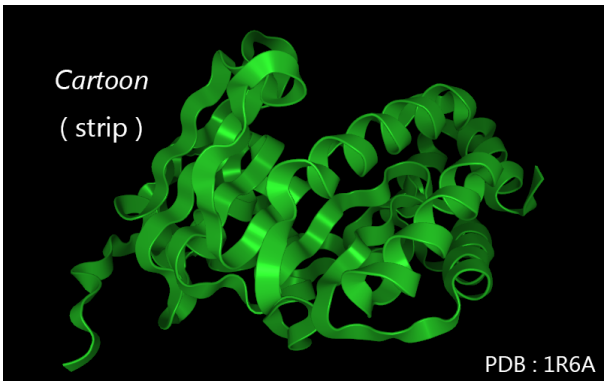
(f) Cartoon



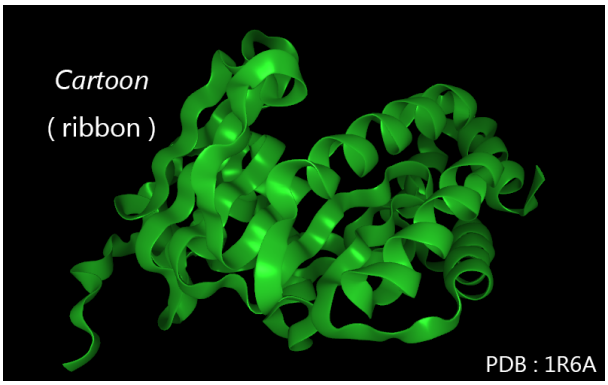
(g) Cartoon - Putty



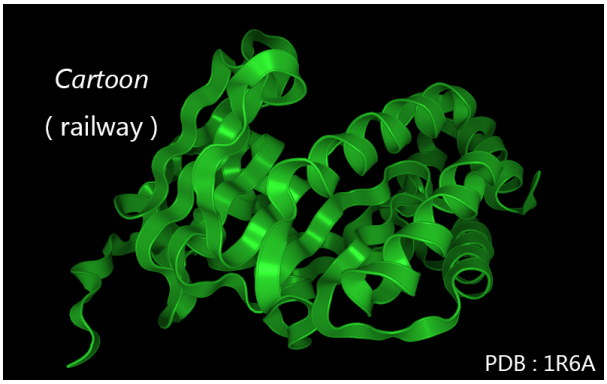
(h) Cartoon - Cube



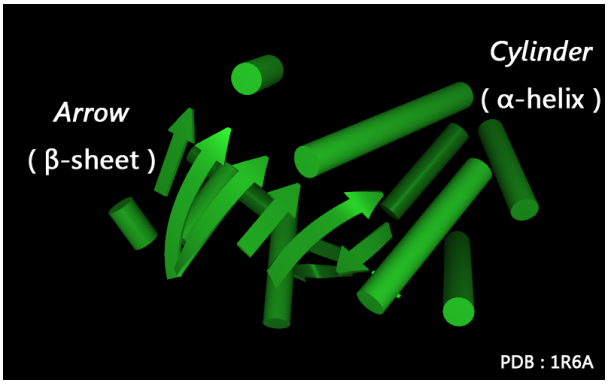
(i) Cartoon - Strip



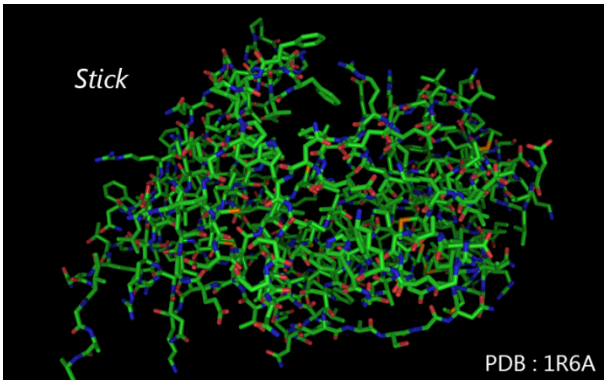
(j) Cartoon - Ribbon



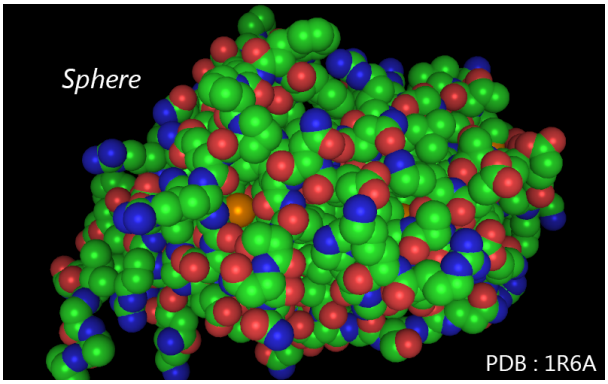
(k) Cartoon - Railway



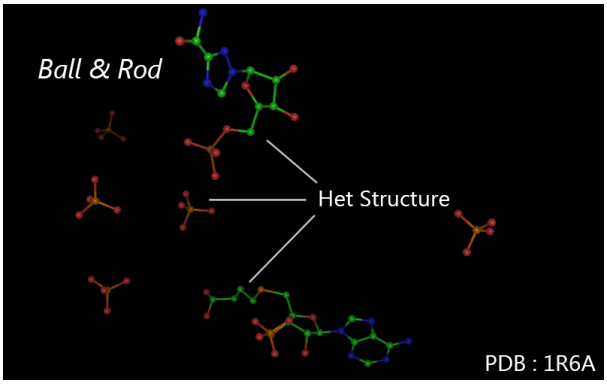
(l) Cartoon – Cylinder & Arrow



(m) Stick



(n) Sphere



(o) Ball & Rod

Figure 4. Representation Mode

Color Mode

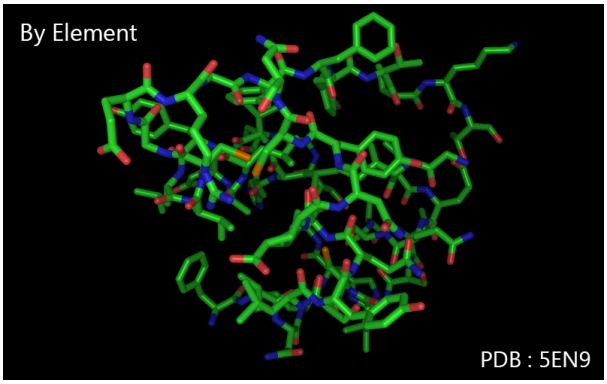
Color mode can be adjusted in Color Plane.

Color Scheme can be adjusted in Configuration Plane, also see *Color Scheme* department.

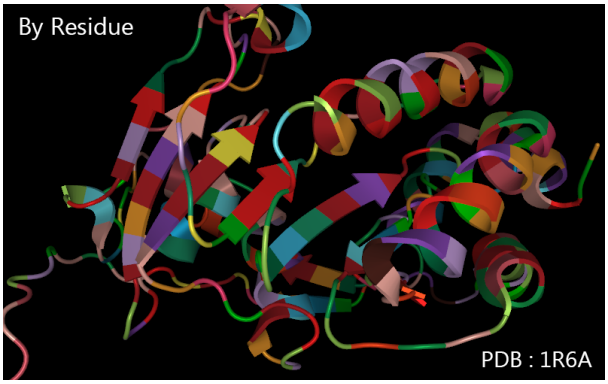
By Element	Color by element.
By Residue	Color by residue.
By Secondary Structure	Color by the secondary structure.
By Chain	Color by chain identifier.
By Representation	Color by representation modes.
By B-Factor	Color as a spectrum according to B-Factor. (high -> low ~~ red -> purple)
By Spectrum	Color as a spectrum according to atoms' serial number (little -> great ~~ red -> purple)
By Chain Spectrum	Color as a spectrum according to residues' sequence number in a chain. (N-end -> C-end ~~ red -> purple)
By Hydrophobicity	Color as a spectrum according to residues' hydrophobicity (Hydrophobic -> Hydrophilic ~~ red -> blue)

By User Defined Color by user.

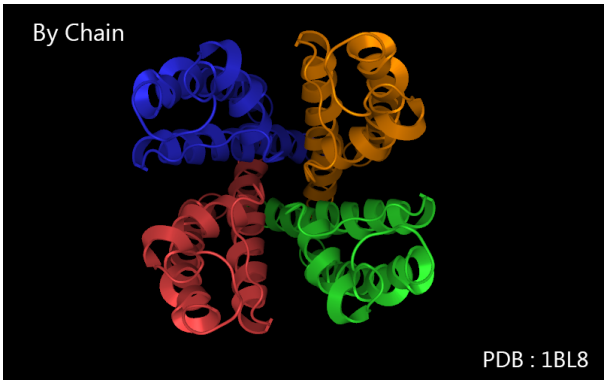
(NOTE : Only available in Fragments customization.)



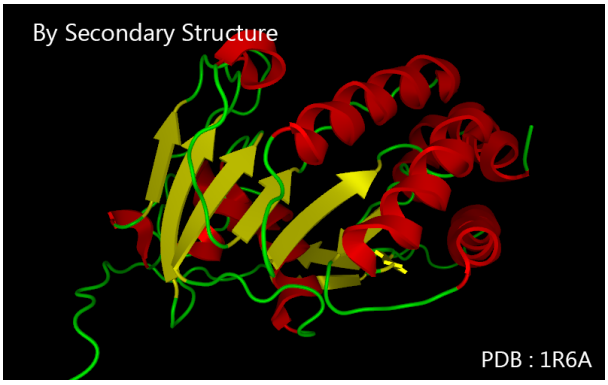
(a) By Element



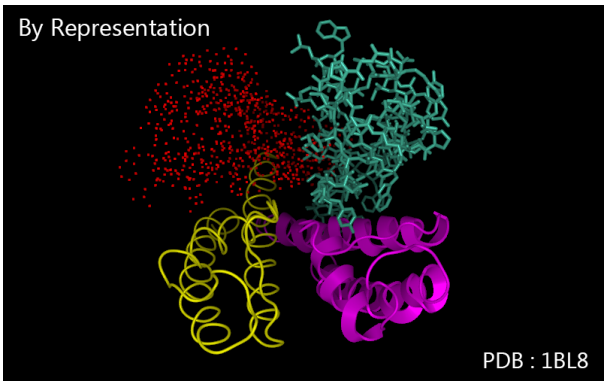
(b) By Residue



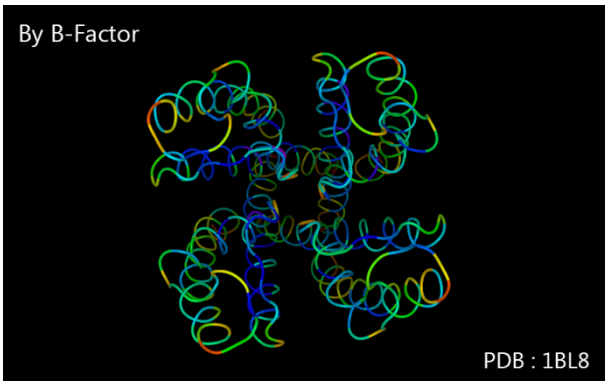
(c) By Chain



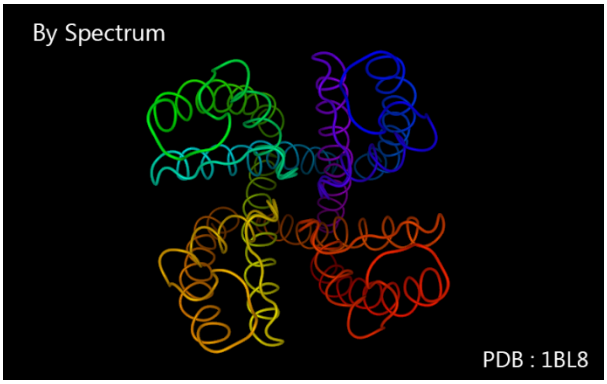
(d) By Secondary Structure



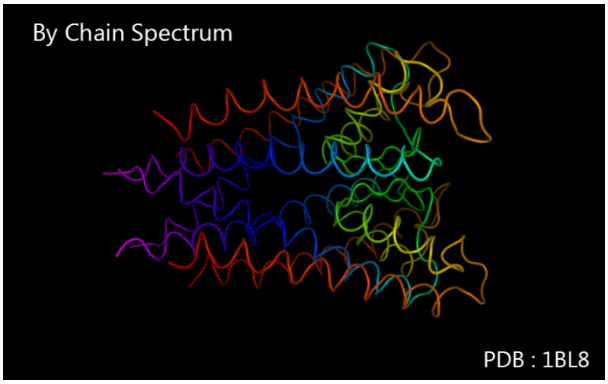
(e) By Representation



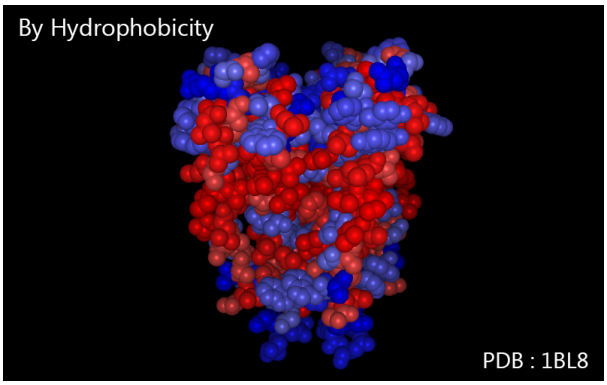
(f) By B-Factor



(g) By Spectrum



(h) By Chain Spectrum



(i) By Hydrophobicity

Figure 5. Color Mode

Label

There are two dimensions for label:

Label Area	What will be labeled.
Label Content	What will be labeled with.

Label Area & *Label Content* can be adjusted in Label Plane.

Label's color and size can be adjusted in Configuration Plane.

Label Area

None	Label nothing.
Every Atom	Label every atom.
Backbone	Label atoms in the main chain.
Every Residue	Label representative atom of every residue.
Every Chain	Label the first atom of every chain.
Mol	Label the first atom of the molecule.

Label Content

Atom name	Label with atom name. (eg. Ca)
Atom id	Label with atom serial number.
Atom name & id	Label with atom name and atom serial number. (eg. Ca-20)
Element	Label with element name.
Element & id	Label with element name and atom serial number. (eg. C-20)
Residue name	Label with residue name. (eg. Tyr)
Residue id	Label with residue sequence number.
Residue name & id	Label with residue name and residue sequence number. (eg. Try45)
Chain id	Label with chain identifier.
Chain & Residue	Label with chain identifier, residue name and residue sequence number. (eg. A.Try45)
Chain & Residue id	Label with chain identifier and residue sequence number. (eg. A.45)
Mix Info	Label with chain identifier, residue name, residue sequence number and atom name. (eg. A.Try45-Ca)
Occupancy	Label with the atom's occupancy recorded in PDB file.
B-Factor	Label with the atom's b-factor recorded in PDB file.
VDW Radius	Label with the atom's van der Waals radius.

Fragment

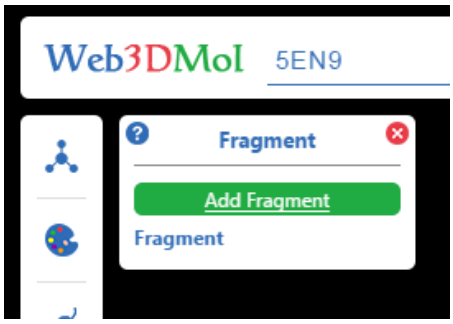
A fragment is a segment of a chain in a molecule.

Fragments can be *added*, *highlighted* and *hidden* in Fragment Plane.

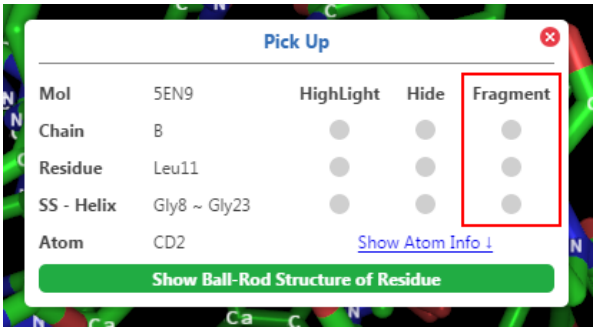
Fragments can be *customized* and *deleted* in Fragment Dialog.

How to add a fragment? (three ways)

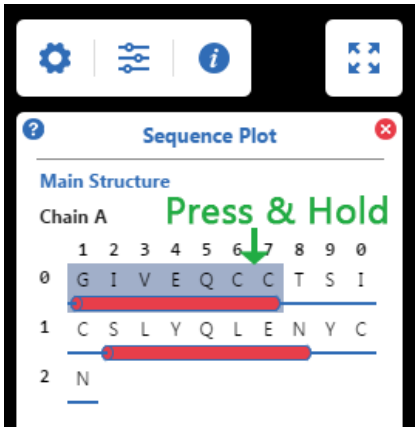
1. Click **Add Fragment** button in Fragment Plane.



2. Click **Fragment** checkboxes in Pickup Dialog to add the chain, residue or secondary structure as fragments.



3. Hover above the sequence plot in Sequence Plane to recognize a piece of sequence, then Press and Hold **left** mouse for a few seconds.



Customization Option

A fragment has its own representation mode, color mode, label area and label content, which can be customized by users in Fragment Dialog.

Chain ID	The chain identifier of a fragment.
Residue Start	The first residue of a fragment.
Residue Stop	The last residue of a fragment.
Representation	The representation mode of a fragment.
Color	The color mode of a fragment. User-defined color is available.
Label Area	The label area of a fragment.
Label Content	The label content of a fragment.

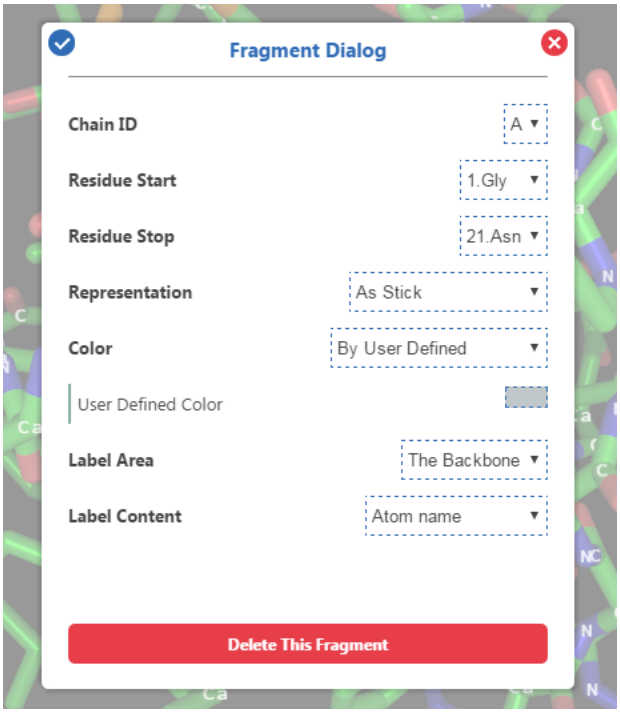


Figure 6. Fragment Dialog

Highlight, Hide & Delete

Highlight	LEFT click the banner of Fragment List in Fragment Plane

Hide	RIGHT click the banner of Fragment List in Fragment Plane
Delete	Click Delete button in Fragment Dialog

Measure

User can measure *Distance*, *Vector Angle*, *Dihedral Angle* and *Triangle Area* in Measure Plane.

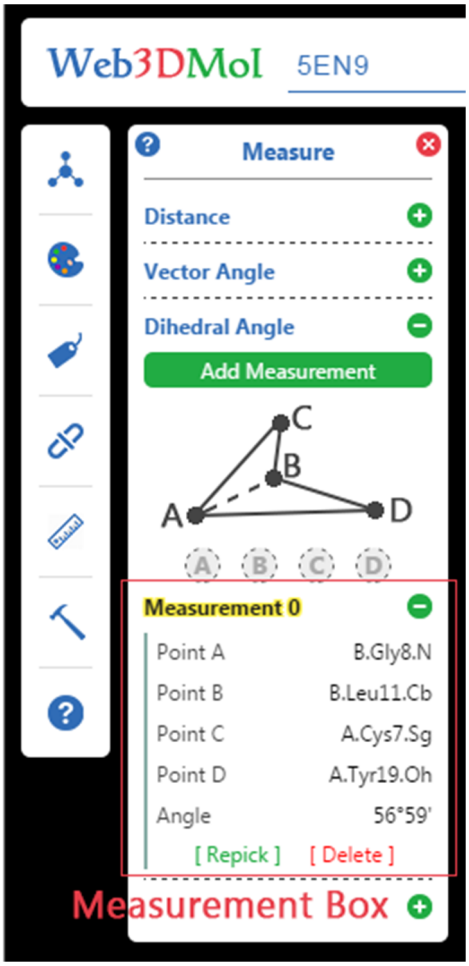


Figure 7. Measure Plane

Processes of Measurement

(1) Click ***Add Measurement*** button in Measure Plane.

(2) ***Left*** click the 3D structure to pick atoms order by *A*, *B*, *C* and *D*.

(3) When points are enough, the result will be calculated and show in Measurement Box. Guide lines and Result label will be added to 3D structure graphics.

(4) Points can be repicked by clicking [***Repick***] in Measurement Box. Click the banner of Measurement Box to show or hide the guide lines of this measurement. Other adjustment options can be found in Configuration Plane - Misc Category.

Tools

Several tools are available in Tool Plane.

Extra Structure

Some extra structures can be added into canvas, including:

Disulfide bonds	The disulfide bonds between cysteines
Cell unit	The cell unit in crystallography
Water molecules	The water molecules in Het structure

Animation

3D structure in canvas can rotate by X, Y, Z axes automatically.

The speed of rotation can be adjusted in Configuration Plane - Misc Category.

Snapshot

3D structure in canvas can be saved as PNG / JPG / BMP pictures.

Share

Click ***Share URL*** and copy the URL shown in Share Dialog.

Pass this URL to others or embed it into a web page.

Pickup

Users can pick atoms by RIGHT clicking the 3D structure.

- Some information about the picked atom is listed in a pop-up dialog, including: *PDB-ID*, *chain identifier*, *residue*, *secondary structure*, *atom's serial number*, *name*, *coordinate*, *occupation* and *b-factor*.
- Ball-Rod structure of the residue can be shown by clicking ***Show Ball-Rod Structure of Residue*** button in the dialog.
- The chain, residue and secondary structure can be highlighted or hidden by clicking ***Highlight / Hide*** checkboxes in the dialog.
- The chain, residue and secondary structure can be added to a fragment by clicking ***Fragment*** checkboxes in the dialog.

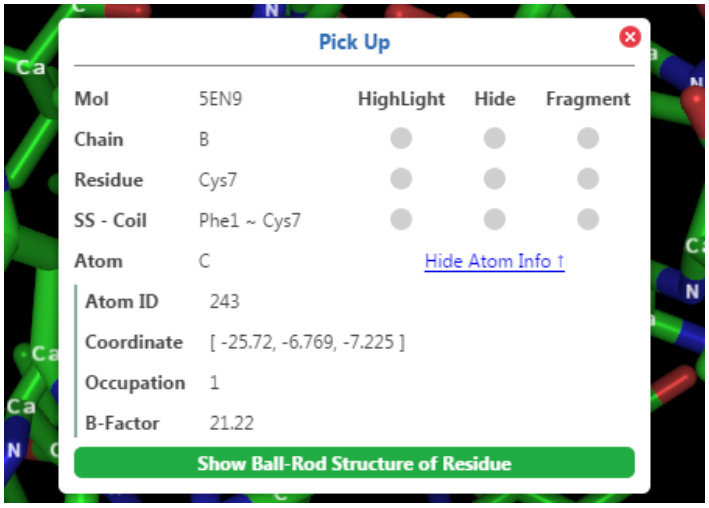


Figure 8. Pickup Dialog

Configuration

Default configurations can be adjusted in Configuration Plane.

Following configurations are listed by this format:

Configuration Name Configuration Key Configuration Description

Geometry

Initial Size geom_mol_size The initial size of 3D structure

Dot Size geom_dot_size Size of point in Dot Rep.

Dot as Cross geom_dot_as_cross Show cross instead of point in Dot Rep.

Dot Cross Radius geom_cross_radius Radius of cross in Dot Rep.

Dash Line Gap geom_dash_gap Gap width of dash line

Backbone as Tube geom_backbone_as_tube

Use tubes instead of lines to connect atoms in Backbone Rep.

Tube Smooth geom_tube_smooth

Use smooth curve instead of polygonal lines in Tube Rep.

Tube Radius geom_tube_radius

Radius of tube in Tube Rep. & Cartoon Rep.

Tube Round End geom_tube_round

Use spheres instead of plains at each ends of the tube in Tube Rep.

Stick Radius geom_stick_radius Radius of tube in Stick Rep.

Stick Round End geom_stick_round

Use spheres instead of plains at each ends of the tube in Stick Rep.

Helix Mode geom_helix_mode

The representation mode of α-helix in Cartoon Rep.

Helix Side Differ geom_helix_side_differ

Fill the side face of α-helix with different color in Cartoon Rep.

Helix Side Color geom_helix_side_color

The different color for side face of α-helix in Cartoon Rep.

Helix Inner Differ geom_helix_inner_differ

Fill the inner face of α-helix with different color in Cartoon Rep.

Helix Inner Color geom_helix_inner_color

The different color for inner face of α-helix in Cartoon Rep.

Sheet Mode geom_sheet_mode

The representation mode of β-sheet in Cartoon Rep.

Sheet Flat geom_sheet_flat

Flatten the β-sheet in Cartoon Rep.

Sheet Side Differ geom_sheet_side_differ

Fill the side face of β-sheet with different color in Cartoon Rep.

Sheet Side Color geom_sheet_side_color

The different color for side face of β-sheet in Cartoon Rep.

Loop Mode geom_loop_mode

The representation mode of random coil in Cartoon Rep.

Putty Radius Min geom_putty_radius_min

The minimum radius of tube in Cartoon-Putty Rep.

Putty Radius Max geom_putty_radius_max

The maximum radius of tube in Cartoon-Putty Rep.

Cube Width geom_cube_width

The width of the cross section in Cartoon-Cube Rep.

Cube Height geom_cube_height

The height of the cross section in Cartoon-Cube Rep.

Cube Side Differ geom_cube_side_differ

Fill the side face with different color in Cartoon-Cube Rep.

Cube Side Color geom_cube_side_color

The different color for side face in Cartoon-Cube Rep.

Strip Width geom_strip_width

The width of the cross section in Cartoon-Strip Rep.

Strip Height geom_strip_height

The height of the cross section in Cartoon-Strip Rep.

Strip Side Differ geom_strip_side_differ

Fill the side face with different color in Cartoon-Strip Rep.

Strip Side Color geom_strip_side_color

The different color for side face in Cartoon-Strip Rep.

Ribbon Width geom_ribbon_width

The width of the cross section in Cartoon-Ribbon Rep.

Ribbon Height geom_ribbon_height

The height of the cross section in Cartoon-Ribbon Rep.

Ribbon Side Height geom_ribbon_side_height

The height of the side face in Cartoon-Ribbon Rep.

Ribbon Side Differ geom_ribbon_side_differ

Fill the side face with different color in Cartoon-Ribbon Rep.

Ribbon Side Color geom_ribbon_side_color

The different color for side face in Cartoon-Ribbon Rep.

Railway Width geom_railway_width

The width of the cross section in Cartoon-Railway Rep.

Railway Height geom_railway_height

The height of the cross section in Cartoon-Railway Rep.

Railway Radius geom_railway_radius

The radius of the side track in Cartoon-Railway Rep.

Railway Side Differ geom_railway_side_differ

Fill the side track with different color in Cartoon-Railway Rep.

Railway Side Color geom_railway_side_color

The different color for side track in Cartoon-Railway Rep.

Arrow Width geom_arrow_width

The width of the cross section in Cartoon-Arrow Rep.

Arrow Height geom_arrow_height

The height of the cross section in Cartoon-Arrow Rep.

Arrowhead Lower Width geom_arrowhead_lower

The width of arrowhead trapezoid's lower face in Cartoon-Arrow Rep.

Arrowhead Upper Width geom_arrowhead_upper

The width of arrowhead trapezoid's upper face in Cartoon-Arrow Rep.

Arrow Side Differ geom_arrow_side_differ

Fill the side face with different color in Cartoon-Arrow Rep.

Arrow Side Color geom_arrow_side_color

The different color for side face in Cartoon-Arrow Rep.

Cylinder Radius geom_cylinder_radius

The radius of tube in Cartoon-Cylinder Rep.

Cylinder Round End geom_cylinder_round_end

Use spheres instead of plains at each ends of the tube in Cartoon-Cylinder Rep.

Cylinder End Differ geom_cylinder_end_differ

Fill the end face with different color in Cartoon-Cylinder Rep.

Cylinder End Color geom_cylinder_end_color

The different color for end face in Cartoon-Cylinder Rep.

Sphere Radius geom_sphere_radius

The radius of sphere in common Reps, rather than Sphere Rep.

Ball Radius geom_ball_radius The radius of ball in Ball & Rod Rep.

Rod Radius geom_rod_radius The radius of rod in Ball & Rod Rep.

Smooth

Segment of Path smooth_segment

The segment number between two guide points in smooth curve path.

(NOTE : Increase this option's value will make nicer graphics but consume more computational resources.)

Curvature of Path smooth_curvature

The curvature of smooth curve path.

(NOTE : Increase this option's value will make the path more twisting.)

Color

Default color scheme can be modified in this category.

(Also see *Color Scheme department*)

Light

Light Enable light_enable Enable light effect

Light Mode light_mode The mode of light effect (Point / Parallel)

Light Position light_position

The position of point light. (Only available for Point Light Mode)

Light Direction light_direction

The direction of parallel light. (Only available for Parallel Light Mode)

Light Color light_color The color of light

Light Ambient light_ambient The color of ambient light

Fog

Fog Enable fog_enable Enable fog effect

Fog Mode fog_mode The mode of fog effect (Linear / Exponential)

Fog Start fog_start

The distance from the camera where the fog starts (fog concentration: 0%)

Fog Stop fog_stop

The distance from the camera where the fog stops (fog concentration: 100%)

Fog Color fog_color The color of fog

Fog Density fog_density

The density of fog. (Only available for Exponential Fog Mode)

Material

Ambient Coefficient material_ambient

Material's weighting coefficient of ambient light

Diffuse Coefficient material_diffuse

Material's weighting coefficient of diffuse light

Ambient Coefficient material_specular

Material's weighting coefficient of specular light

Shininess Exponent material_shininess

Material's shininess exponent of specular light

Label

Label Size label_size Font size of label

Label Color label_color Color of label

Speed

Mouse Rotate Speed rotate_speed

Speed of rotation movement while mouse interaction

Mouse Zoom Speed zoom_speed

Speed of zoom movement while mouse interaction

Mouse Translate Speed pan_speed

Speed of translation movement while mouse interaction

Animation Speed animation_speed

Speed of rotation movement while animation

Misc

Background bg Background color of the canvas

Show Measurement show_measurement

Show guide lines and measurement result in canvas.

Measure Line Color measure_line_color

Color of guide lines in measurement

Measure Angle in Radian measure_angle_in_radian

Use radian instead of degree in measurement.

Label Ball & Rod label_ball_and_rod

Label every atom of Ball & Rod Rep. in fragments customization.

Local Storage

If local storage is enabled, next time you initialize Web3DMol, configuration values saved at local storage will take place of default one.

Recover Default Config Recover the default configuration values

Save Config to Local	Save current configuration values to local storage
Recover Config from Local Storage	Recover configuration value from local storage
Clear Local Storage	Clear configuration values saved at local storage

Representation Mode (listed in Representation Plane) (Also see *Representation department*)

Rep Mode Main	rep_mode_main	Representation Mode for Main Structure
Rep Mode Het	rep_mode_het	Representation Mode for Het Structure

NOTE: values are limited in following integers.

100 (Hide)	*101 (Dot)*	*102 (Line)*
103 (Backbone)	*104 (Tube)*	*105 (Cartoon)*
106 (Cartoon - Putty)	*107 (Cartoon - Cube)*	*108 (Cartoon - Strip)*
109 (Cartoon - Ribbon)	*110 (Cartoon - Railway)*	*111 (Cartoon - Arrow)*
112 (Cartoon - Cylinder)	*113 (Stick)*	*114 (Sphere)*
115 (Ball & Rod)		

Color Mode (listed in Color Plane) (Also see *Color department*)

Color Mode Main	color_mode_main	Color Mode for Main Structure
Color Mode Het	color_mode_het	Color Mode for Het Structure

NOTE: values are limited in following integers.

601 (By Element)	*602 (By Residue)*	*603 (By Secondary Structure)*
604 (By Chain)	*605 (By Representation)*	*606 (By B-Factor)*
607 (By Spectrum)	*608 (By Chain Spectrum)*	*609 (By Hydrophobicity)*

Label Area (listed in Label Plane) (Also see *Label department*)

Label Area Main	label_area_main	Label Area for Main Structure
Label Area Het	label_area_het	Label Area for Het Structure

NOTE: values are limited in following integers.

700 (Label None)	*701 (Label Every Atom)*	*702 (Label Backbone)*
703 (Label Every Residue)	*704 (Label Every Chain)*	*705 (Label Molecule)*

Label Content (listed in Label Plane) (Also see *Label Department*)

Label Content Main	label_content_main	Label Content for Main Structure
Label Content Het	label_content_het	Label Content for Het Structure

NOTE: values are limited in following integers.

711 (Atom name)	*712 (Atom id)*	*713 (Atom name & id)*
721 (Element)	*722 (Element & id)*	
731 (Residue name)	*732 (Residue id)*	*733 (Residue name & id)*
741 (Chain id)	*742 (Chain & Residue)*	*743 (Chain & Residue id)*
744 (Mix Info)		
751 (Occupancy)	*752 (B-Factor)*	*753 (van der Waals Radius)*

Color Scheme

Color mode can be adjusted in *Color Plane*. (Also see *Color department*)

Color Scheme can be adjusted in *Configuration Plane*.

For developers, Color Scheme can be redefined by modifying the ***color*** value in *URL* or passing the ***user_color*** argument in `w3m.api.init()` function. (Also see *Extension department*)

Color Scheme are listed by this format:

Color Scheme Name Color Index Color Value

(NOTE : Color Value is a *JavaScript Array*, like `[1.000,1.000,1.000]`, representing Red, Green, Blue color channels. Each channel's value must be normalized between 0 ~ 1.)

Special Color

Default Color	1	[0.750 , 0.780 , 0.790]
Measure Guide Line	2	[1.000 , 1.000 , 0.000]
Helix Side Color	11	[0.790 , 0.410 , 0.140]
Helix Inner Color	12	[0.750 , 0.750 , 0.750]
Sheet Side Color	13	[0.750 , 0.750 , 0.750]
Cube Side Color	14	[0.790 , 0.410 , 0.140]
Strip Side Color	15	[0.790 , 0.410 , 0.140]
Railway Side Color	16	[0.790 , 0.410 , 0.140]
Ribbon Side Color	17	[0.790 , 0.410 , 0.140]
Arrow Side Color	18	[0.790 , 0.410 , 0.140]
Cylinder End Color	19	[0.790 , 0.410 , 0.140]

Color for Element

C	101	[0.200 , 1.000 , 0.200]
O	102	[1.000 , 0.300 , 0.300]
N	103	[0.180 , 0.180 , 0.930]
S	104	[1.000 , 0.560 , 0.000]
H	105	[0.820 , 0.820 , 0.820]
P	106	[0.790 , 0.410 , 0.140]
Fe	107	[1.000 , 0.275 , 0.122]

Cu	108	[0.086 , 0.663 , 0.318]
Co	109	[0.020 , 0.467 , 0.282]
Zn	110	[1.000 , 0.945 , 0.263]
Mn	111	[0.267 , 0.808 , 0.965]
I	112	[0.800 , 0.643 , 0.890]
Na	113	[0.859 , 0.353 , 0.400]
K	114	[0.086 , 0.522 , 0.663]
Ca	115	[0.129 , 0.651 , 0.459]
Mg	116	[0.851 , 0.714 , 0.067]
Al	117	[0.553 , 0.294 , 0.733]
Cl	118	[0.553 , 0.294 , 0.733]

Color for Residue

Ala	201	[1.000 , 0.275 , 0.122]
Gly	202	[1.000 , 0.702 , 0.655]
Ile	203	[0.859 , 0.353 , 0.400]
Leu	204	[1.000 , 0.129 , 0.129]
Pro	205	[1.000 , 0.278 , 0.467]
Val	206	[0.749 , 0.141 , 0.165]
Phe	207	[0.267 , 0.808 , 0.965]
Trp	208	[0.439 , 0.953 , 1.000]
Tyr	209	[0.086 , 0.522 , 0.663]
Ser	210	[0.086 , 0.663 , 0.318]
Thr	211	[0.000 , 0.737 , 0.071]
Cys	212	[0.129 , 0.651 , 0.459]
Met	213	[0.000 , 0.898 , 0.000]
Asn	214	[0.588 , 0.808 , 0.329]
Gln	215	[0.020 , 0.467 , 0.282]

Asp	216	[1.000 , 0.945 , 0.263]
Glu	217	[1.000 , 0.651 , 0.192]
Arg	218	[0.800 , 0.643 , 0.890]
His	219	[0.298 , 0.133 , 0.106]
Lys	220	[0.553 , 0.294 , 0.733]
A	221	[0.000 , 0.204 , 0.447]
C	222	[0.851 , 0.714 , 0.067]
G	223	[0.459 , 0.259 , 0.400]
U	224	[0.231 , 0.180 , 0.494]
dA	225	[0.294 , 0.361 , 0.769]
dC	226	[0.886 , 0.612 , 0.271]
dG	227	[0.549 , 0.263 , 0.337]
dT	228	[0.667 , 0.298 , 0.561]

Color for Secondary Structure

α-Helix	301	[1.000 , 0.000 , 0.000]
β-Sheet	302	[1.000 , 1.000 , 0.000]
Random Coil	303	[0.000 , 1.000 , 0.000]

Color for Chain

A	401	[0.200 , 1.000 , 0.200]
B	402	[1.000 , 0.300 , 0.300]
C	403	[0.180 , 0.180 , 0.930]
D	404	[1.000 , 0.560 , 0.000]
E	405	[0.540 , 0.360 , 0.540]
F	406	[0.790 , 0.410 , 0.140]
G	407	[0.820 , 0.820 , 0.820]

H	408	[0.086 , 0.522 , 0.663]
I	409	[1.000 , 0.651 , 0.192]
J	410	[0.298 , 0.133 , 0.106]
K	411	[0.859 , 0.353 , 0.400]
L	412	[0.086 , 0.522 , 0.663]
M	413	[0.086 , 0.522 , 0.663]
N	414	[0.851 , 0.714 , 0.067]

Color for Representation Mode

Dot	501	[1.000 , 0.000 , 0.000]
Line	502	[0.000 , 1.000 , 0.000]
Backbone	503	[0.000 , 0.000 , 1.000]
Tube	504	[1.000 , 1.000 , 0.000]
Cartoon	505	[1.000 , 0.000 , 1.000]
Cartoon – Putty	506	[0.000 , 1.000 , 1.000]
Cartoon – Cube	507	[1.000 , 0.275 , 0.122]
Cartoon – Strip	508	[0.267 , 0.808 , 0.965]
Cartoon – Railway	509	[0.086 , 0.663 , 0.318]
Cartoon – Ribbon	510	[1.000 , 0.945 , 0.263]
Cartoon – Arrow	511	[0.800 , 0.643 , 0.890]
Stick	512	[0.282 , 0.753 , 0.639]
Sphere	513	[1.000 , 0.776 , 0.667]
Ball & Rod	514	[0.420 , 0.482 , 0.431]

Sequence

A sequence plot is shown in Sequence Plane.

Secondary Structure in Sequence Plot

Secondary structures and single residues will be recognized automatically when mouse *hovering* over the sequence plot.

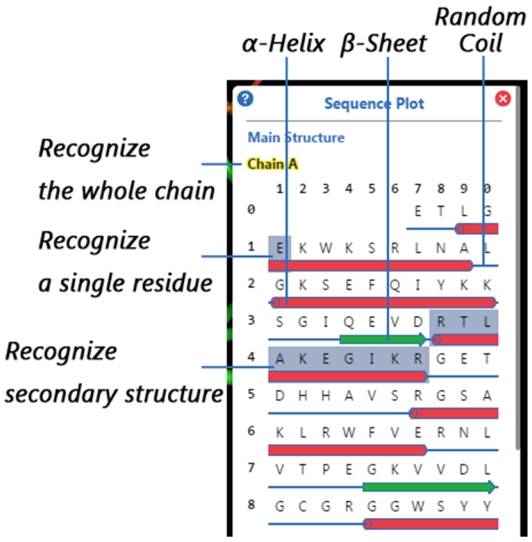


Figure 9. Sequence Plot

α-Helix	shown as small red cylinders.
β-Sheet	shown as small green arrows.
Random Coil	shown as thin blue strips.

Highlight, Hide & Fragment

Hover to recognize a segment, then:

Highlight	Left click to highlight.
Hide	Right click mouse to hide.
Add Fragment	Press & Hold Left mouse for a few seconds to add the recognized segment as a fragment.

Information

Some important information dug out from PDB files is listed in *Information Plane*.

Including:

Molecular Classification, *Title of Experiment*, *Technique of Experiment*, *Source of Organism*, *Structural Resolution*, *Publication*, *Author* etc.

RCSB link of the molecule, *PubMed link* and *DOI link* of the publication are available in Link Category.

Figure 10. Information Plane

Extension

Web3DMol can be embedded into other applications.

A typical URL

```
http://web3dmol.duapp.com/?id=xxxx&widget=x&config=xxxxxx&color=xxxxxx
```

id	required	PDB-id of the molecule to be shown in canvas.
widget	optional	Show the widgets in canvas. (0 : do not show; 1 : show)
config	optional	Modified configuration values. (using ***JSON string***)
color	optional	Modified color values. (using ***JSON string***)

Configuration values & Color values can be modified to customize the 3D structure graphics.

Configuration keys are listed in *Configuration department* in this manual.

Color index are listed in *Color Scheme department* in this manual.

Firstly,

Configuration values & Color values must be formatted as JSON String

We recommend using JSON Tools to produce JSON String, such as `JSON.stringify()` in JavaScript.

Configuration

Format `{ "configuration_key" : configuration_value }`

Example `{ "rep_mode_main" : 105, "color_mode_main" : 602, "bg" : [ 1.0,1.0,1.0,0.0 ] }`

Color

Format `{ "color_index" : color_value }`

Example `{ "1" : [ 0.5,0.5,0.5 ], "102" : [ 0.8,0.8,0.8 ] }`

Next,

Encode the JSON String with URL Encode Tools, such as `encodeURIComponent()` in JavaScript.

The encoded Configuration values will be like:

`%7B%22rep_mode_main%22%3A105%2C%22color_mode_main%22%3A602%2C%22bg%22%3A%5B1%2C1%2C1%2C0%5D%7D`

The encoded Color values will be like:

`%7B%221%22%3A%5B0.5%2C0.5%2C0.5%5D%2C%22102%22%3A%5B0.8%2C0.8%2C0.8%5D%7D`

Finally,

The URL will be like:

`http://web3dmol.duapp.com/?id=1mbs&widget=0&config=%7B%22rep_mode_main%22%3A105%2C%22color_mode_main%22%3A602%2C%22bg%22%3A%5B1%2C1%2C1%2C0%5D%7D&color=%7B%221%22%3A%5B0.5%2C0.5%2C0.5%5D%2C%22102%22%3A%5B0.8%2C0.8%2C0.8%5D%7D`

Using <iframe> in HTML

The typical code:

```
<iframe width=800 height=500 src="{url}" frameborder=0 allowfullscreen></iframe>
```

Obviously, the value of "***src***" should be replaced by a new URL, and the values of "***width***" and "***height***" could be modified in order to fit the whole layout of your web page.

Using JavaScript

Web3DMol's Library must be loaded into your application at first.

Online Library URL -> `http://web3dmol.duapp.com/web3dmol.js`

We recommend developers to download Web3DMol source code and make it a part of your own application to enhance response speed.

The initialization function is defined like:

```
w3m.api.init(div_id, pdb_id, show_widget, user_config, user_color)
```

div_id	required	ID of the container node for Web3DMol in a web page.
pdb_id	required	PDB-id of the molecule to be shown in canvas.

show_widget	optional	Show the widgets in canvas. (0 : do not show; 1 : show)
user_config	optional	Modified configuration values. (using *JavaScript Object*)
user_color	optional	Modified color values. (using *JavaScript Object*)

user_config & *user_color* and both **JavaScript Object** rather than JSON String.

The typical code:

```
<script type="text/javascript" src="http://web3dmol.duapp.com/web3dmol.js"></script>
<script type="text/javascript">
w3m.api.init('app', '1r6a', 1, { user_config }, { user_color });
</script>
```

Using WebView Component

In desktop environment, a WebView Component must be used to embed Web3DMol. For example, in **Qt**, *QtWebView* is the WebView Component. Developers can set the ***url*** attribute of a WebView component with URL we used above, and ensure that the JavaScript Engine in on.

By this way, we can easily embed Web3DMol into a desktop application.

Limitation

3D modeling and rendering are both resource-intensive calculations, and as a form of interpreted language, JavaScript is not good at high efficiency calculations. Therefore, when the size of a molecule becomes very large, Web3DMol sacrifices some graphical quality to maintain the efficiency. Another restriction is from web browser manufacturers. For example, V8, the JavaScript engine in Google Chrome, has a threshold for maximum

heap memory usage, so that when the number of atoms is too large, Chrome will crash. In fact, for very large molecules, RCSB PDB does not offer common PDB archives to download. Instead, structural data are recorded in a more complicated format such as mmCIF. Under these conditions, we recommend use of desktop software, for example PyMOL, whose modeling and rendering algorithms are written in C++ (a compiled language).

JavaScript was originally designed for web page interaction, and its function libraries are not abundant. Therefore, it is difficult for Web3DMol to handle PDB archives if they are in zipped format or to record a small movie while users are manipulating the 3D structure.

The support for WebGL from mobile devices is uneven. Web3DMol runs well on some of the latest cellphones, but not very smoothly on most mobile devices at present. The memory capacity, the performance of microchips and the touch-based interactions limit the user experience of Web3DMol on mobile devices.

API

APIs are for developers who use JavaScript to embed Web3DMol into their applications.

```
w3m.api.init (div_id, pdb_id, show_widget, user_config, user_color)
```

Initialize Web3DMol.

div_id	required	ID of the container node for Web3DMol in a web page.
pdb_id	required	PDB-id of the molecule to be shown in canvas.
show_widget	optional	Show the widgets in canvas. (0 : do not show; 1 : show)
user_config	optional	Modified configuration values. (using JavaScript Object)
user_color	optional	Modified color values. (using JavaScript Object)

```
w3m.api.config (key, value)
```

Set or Get configuration.

if value is undefined, get and return the configuration value, if value is defined, set the configuration value. (also see *Configuration department*)

key	required	The configuration key.
value	optional	The configuration value.

`w3m.api.rgb (index, value)`

Set or Get color value.

if value is undefined, get and return the color value, if value is defined, set the color value. (also see *Color Scheme department*)

index	required	The color index in color scheme.
value	optional	The color value (a JavaScript array).

`w3m.api.refresh ()`

Refresh the background and the graphics.

`w3m.api.pdb (source)`

Load a PDB file from a PDB-ID or a local file.

source	required	A PDB id or a file user selected from <input type="file" />

`w3m.api.representation (structure, mode)`

Switch the representation mode.

structure	required	1 : main structure; 2 : het structure
mode	required	See *Configuration department - Representation category*.

w3m.api.color (structure, mode)

Switch the color mode.

structure	required	1 : main structure; 2 : het structure
mode	required	See *Color Scheme department*.

w3m.api.label_area (structure, area)

Switch the label area.

structure	required	1 : main structure; 2 : het structure
mode	required	See *Configuration department - Label Area category*.

w3m.api.label_content (structure, content)

Switch the label content.

structure	required	1 : main structure; 2 : het structure
mode	required	See *Configuration department - Label Content category*.

w3m.api.fragment_add (chain_id, start, stop)

Add a fragment. This function will return the fragment id of this fragment.

chain_id	optional	The chain identifier of this fragment.
start	optional	The first residue of this fragment.
stop	optional	The last residue of this fragment.

w3m.api.fragment_set (fragment_id, rep_mode, color_mode, label_area, label_content, color_defined)

Customize a fragment.

fragment_id	required	Id of the fragment which will be customized.
rep_mode	required	The representation mode of this fragment.
color_mode	required	The color mode of this fragment.
label_area	required	The label area of this fragment.
label_content	required	The label content of this fragment.
color_defined	required	The used defined color of this fragment.

(Taking effect only when color mode is COLOR_BY_USER.)

w3m.api.fragment_remove (fragment_id)

Remove a fragment.

fragment_id	required	Id of the fragment which will be removed.

w3m.api.highlight_add (chain_id, start, stop)

HighLight a segment.

chain_id	required	The chain identifier of this segment.
start	required	The first residue of this segment.
stop	required	The last residue of this segment.

w3m.api.highlight_remove (chain_id, start, stop)

Remove the HighLight effect of a segment.

chain_id	required	The chain identifier of this segment.
start	required	The first residue of this segment.
stop	required	The last residue of this segment.

w3m.api.hide_add (chain_id, start, stop)

Hide a segment.

chain_id	required	The chain identifier of this segment.
start	required	The first residue of this segment.
stop	required	The last residue of this segment.

```
w3m.api.hide_remove (chain_id, start, stop)
```

Remove the Hide effect of a segment.

chain_id	required	The chain identifier of this segment.
start	required	The first residue of this segment.
stop	required	The last residue of this segment.

```
w3m.api.picked ()
```

Return the serial number of the atom picked from the 3D structure by user just now.

```
w3m.api.atom (atom_id)
```

Return the information of an atom.

atom_id	required	The serial number of the atom.

The returned value is a *JavaScript array*:

`[ structure_type, atom_id, atom_name, residue_name, chain_id, residue_id, coordinate, occupancy, b-factor, element ]`.

structure_type	1 : Main Structure, 2 : Het Structure.
coordinate	A JavaScript array: [x, y, z].

Faq

See ***FAQ page***. (http://web3dmol.duapp.com/faq.html)

Example

See ***Example page***. (http://web3dmol.duapp.com/example.html)