



PROTEOPEDIA
— LIFE IN 3D —

A powerful tool for biomolecular
communication
and a 3D encyclopedia of biomolecules

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Visit Proteopedia's main page: <http://proteopedia.org>

Let's explore!



Hands-on:

1. Go to <http://proteopedia.org> and type '**Hemoglobin**' in the empty white search box on the left-hand toolbar, then press 'Go'.
2. Explore the first section. Stop before '**Hemoglobin subunit binding O2**'

Let's explore!



Hands-on:

1. Now type '**Peptide**' in the empty white search box on the left hand toolbar and press 'Go'. Explore this page.

Let's explore!



Hands-on:

1. Navigate back to the '**Main Page**' by clicking the link '**Main Page**' on the left-hand toolbar.
2. Scroll down to '**What can Proteopedia do for me**' and in the '**Educators**' column, click on the link '**tutorials or molecular scenes**', you will be taken to a new page.
3. Now click on the link titled '**Structural_Templates**'
4. Scroll down to the section titled '**Secondary structure elements**'.
5. Explore this section, but stop before the section titled '**Turns and loops**'

STOP (PAUSE) HERE



WHAT ARE WE GOING TO LEARN?

- How to create your own pages in Proteopedia, including 3D structures and green scene links.

HOW TO EDIT A PAGE (1)

Hands-on:

1. Go to <http://proteopedia.org>
2. Use the search box to get to your assigned Sandbox page.
3. You will need to log in to edit the page. **Log in with a guest account.**
4. On your assigned Sandbox page, click on “edit this page”.
5. Then scroll down and click the “save page” button. This will ‘create’ and save your Sandbox page for further editing..

HOW TO EDIT A PAGE (2)

- Your page should now look like this:

The screenshot shows a Proteopedia article page for 'Sandbox 780'. The page layout includes a top navigation bar with tabs for 'article', 'discussion', 'edit this page', 'history', 'protect', 'delete', 'move', and 'watch'. The user 'Joel L. Sussman' is logged in. The page title is 'Sandbox 780' with an '[edit]' link. Below the title is a heading 'Your Heading Here (maybe something like 'Structure')' with an '[edit]' link. The main content area contains a default text block, a 'Contents' table of contents, and sections for 'Function', 'Disease', 'Relevance', and 'Structural highlights'. A 3D protein structure is displayed on the right side, rendered with a blue ribbon and a transparent representation. Below the structure are controls for 'toggle spin', 'toggle quality', and 'popup', along with the 'JSmol' logo. The 'References' section at the bottom contains a single reference: '1. ↑ Hanson, R. M., Prilusky, J., Renjian, Z., Nakane, T. and Sussman, J. L. (2013), JSmol and the Next-Generation Web-Based Representation of 3D Molecular Structure as Applied to Proteopedia. Isr. J. Chem., 53:207-216. doi:http://dx.doi.org/10.1002/ijch.201300024'. The left sidebar features the Proteopedia logo, navigation links (Main Page, Table of Contents, Structure Index, Random, Recent Changes, Help), a search box, and a toolbox with links for exporting, linking, and uploading files.

article discussion **edit this page** history protect delete move watch

Joel L. Sussman my talk my preferences my watchlist my contributions log out

1 open e-mail-confirmed account request pending

Sandbox 780

Your Heading Here (maybe something like 'Structure') [edit]

This is a default text for your page **Sandbox 780**. Click above on **edit this page** to modify. Be careful with the < and > signs.

You may include any references to papers as in: the use of JSmol in Proteopedia ^[1] or to the article describing Jmol ^[2] to the rescue.

Contents [hide]
1 Function
2 Disease
3 Relevance
4 Structural highlights

Function

Disease

Relevance

Structural highlights

This is a sample scene created with SAT to **color** by Group, and another to make a **transparent representation** of the protein. You can make your own scenes on SAT starting

References

1. ↑ Hanson, R. M., Prilusky, J., Renjian, Z., Nakane, T. and Sussman, J. L. (2013), JSmol and the Next-Generation Web-Based Representation of 3D Molecular Structure as Applied to Proteopedia. Isr. J. Chem., 53:207-216. doi:http://dx.doi.org/10.1002/ijch.201300024

toggle spin toggle quality popup JSmol

Caption for this structure

HOW TO EDIT A PAGE (3)

Hands-on:

1. Open a new browser window and navigate to the page “Sandbox” (with no additional number) in Proteopedia.
2. Click on the link to reach an example page on Green Fluorescent Protein. We will recreate this page in Proteopedia as an example.
http://proteopedia.org/w/User:Joel_L._Sussman/GFP_Test_Page
-- keep this page open throughout the workshop.
3. Select the two paragraphs of text, and copy them (ctrl-v). Start from “Green Fluorescent Protein...” and include the heading “Exploring the Structure” as well as both paragraphs.
4. Go back to the browser window with your assigned Sandbox page (the one you cleared earlier), and click “edit this page”.
5. Insert a blank line just after the automatic text on that page that ends with ‘...to the rescue’
6. After the blank line, paste the text that you copied in step (3). Save using the “Save page” button.

HOW TO EDIT A PAGE (5)

- Your page should now look like this (after editing)

The screenshot displays the Proteopedia 'Editing Sandbox 780' page. The browser address bar shows the URL: `www.proteopedia.org/wiki/index.php?title=Sandbox_780&action=edit`. The page title is 'Editing Sandbox 780'. The user is identified as 'Joel L. Sussman'. The page has a navigation bar with tabs for 'article', 'discussion', 'edit this page', 'history', 'protect', 'delete', 'move', and 'watch'. The main content area contains a rich text editor with a toolbar and a text area. The text area contains the following content:

```
==Your Heading Here (maybe something like 'Structure')==  
<StructureSection load='1stp' size='340' side='right' caption='Caption for this structure' scene=''>  
This is a default text for your page "Sandbox 780". Click above on "edit this page" to modify. Be careful with the &lt; and &gt; signs.  
You may include any references to papers as in: the use of JSmol in Proteopedia <ref>DOI:10.1002/ijch.201300024</ref> or to the article describing Jmol <ref>PMID:21638687</ref>  
to the rescue.
```

Green fluorescent protein (GFP), originally isolated from the jellyfish *Aequorea victoria* (PDB entry 1ema), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement.

Exploring the Structure

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The chromophore, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of three residues in the central alpha helix: -Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation creates the chromophore's five-membered ring via a new bond between the threonine and the glycine residues.[1]

```
== Function ==  
== Disease ==  
== Relevance ==
```

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 **SAT (Scene Authoring Tools) [show]**

Summary:

HOW TO EDIT A PAGE (6)

- Your page should now look like this:

The screenshot shows a Proteopedia article page for 'Sandbox 780'. The page layout includes a top navigation bar with user links (Joel L. Sussman, my talk, my preferences, my watchlist, my contributions, log out) and article actions (article, discussion, edit this page, history, protect, delete, move, watch). The main content area features a heading 'Your Heading Here (maybe something like 'Structure')' with an [edit] link. Below the heading is a text box containing a default message: 'This is a default text for your page **Sandbox 780**. Click above on **edit this page** to modify. Be careful with the < and > signs. You may include any references to papers as in: the use of JSmol in Proteopedia [1] or to the article describing Jmol [2] to the rescue.' To the right of the text is a JSmol viewer showing a 3D ribbon structure of a protein (GFP) in light blue, with a yellow and red chromophore. Below the viewer are controls for 'toggle spin', 'toggle quality', and 'popup', along with the JSmol logo and a caption placeholder 'Caption for this structure'. On the left side, there is a sidebar with the Proteopedia logo, navigation links (Main Page, Table of Contents, Structure Index, Random, Recent Changes, Help), a search box, and a toolbox (Export this page, What links here, Related changes, Upload file, Special pages, Printable version, Permanent link). At the bottom of the main content area, there is a 'References' section with a [edit] link and a 'Contents [hide]' section listing '1 Function'.

ADDING SECTION HEADINGS

Hands-on:

1. In your assigned Sandbox page, now displaying your new text, click “edit this page”.
2. We want to make “Introduction” and “Exploring the Structure” as a section headings.
3. Type the text “Introduction” just before the words: “Green fluorescent protein (GFP),” and select the button from the toolbar above the text-editing area with a big “A”.
4. The result should be two equals signs on either side of the words “Introduction”. It should look like this: **==Introduction==**.
5. In a similar way type, add a heading: “Exploring the Structure”, just before “GFP is a beta barrel protein with 11 beta sheets...”
6. Delete the headings: Function, Disease, Relevance, Structural highlights
7. Save the page using the “Save page” button.



ADDING SECTION HEADINGS

- Your page should now look like this:

Joel L. Sussman my talk my preferences my watchlist my contributions log out

article discussion edit this page history protect delete move watch 1 open e-mail-confirmed account request pending

Editing Sandbox 780

B **A**

==Your Heading Here (maybe something like 'Structure')==
<StructureSection load='1stp' size='340' side='right' caption='Caption for this structure' scene=''>
This is a default text for your page '''Sandbox 780'''. Click above on '''edit this page''' to modify. Be careful with the < and > signs.
You may include any references to papers as in: the use of JSmol in Proteopedia <ref>DOI 10.1002/ijch.201300024</ref> or to the article describing Jmol <ref>PMID:21638687</ref> to the rescue.

== Introduction ==

Green fluorescent protein (GFP), originally isolated from the jellyfish *Aequorea victoria* (PDB entry 1ema), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement.

Exploring the Structure

== Exploring the Structure ==

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The chromophore, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of three residues in the central alpha helix: -Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation creates the chromophore's five-membered ring via a new bond between the threonine and the glycine residues.[1]

This is a sample scene created with SAT to <scene name="/12/3456/Sample/1">color</scene> by Group, and another to make <scene name="/12/3456/Sample/2">a transparent

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SAT (Scene Authoring Tools) [show]

Summary:

Your page should now look like this:



PROTEOPEDIA
— LIFE IN 3D —

navigation

- Main Page
- Table of Contents
- Structure Index
- Random
- Recent Changes
- Help

search

Go Search

toolbox

- Export this page
- What links here
- Related changes
- Upload file
- Special pages
- Printable version
- Permanent link

Joel L. Sussman my talk my preferences my watchlist my contributions log out

article discussion edit this page history protect delete move watch

1 open e-mail-confirmed account request pending

Sandbox 780

Your Heading Here (maybe something like 'Structure') [\[edit\]](#)

This is a default text for your page **Sandbox 780**. Click above on **edit this page** to modify. Be careful with the < and > signs.

You may include any references to papers as in: the use of JSmol in Proteopedia ^[1] or to the article describing Jmol ^[2] to the rescue.

Introduction

Green fluorescent protein (GFP), originally isolated from the jellyfish *Aequorea victoria* (PDB entry 1ema), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement. Exploring the Structure

Exploring the Structure

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References

[\[edit\]](#)



[JSmol](#)

toggle spin toggle quality popup

Caption for this structure

15

BOLD AND INTERWIKI LINKS

Hands-on:

1. In your assigned Sandbox page, now displaying your new text, click “edit this page”.
2. We want to make the word “GFP” bold. Select the word “GFP” and click on the button in the toolbar above the text-editing area with a big “B”.
3. The result should be three single quotation marks on either side of the word “GFP” like so: **'''GFP'''**
4. Now make “1ema” into an interwiki link, so that it leads to the Proteopedia page for the PDB entry 1ema. Do this by selecting the text “1ema” and clicking on the button in the toolbar above the text-editing area with a big, underlined, blue “Ab”.
5. The result should be two square inward facing brackets on either side of the word “1ema”. It should look like this: **[[1ema]]**
6. Save the page using the “Save page” button.



Your page should now look like this:

PROTEOPEDIA
— LIFE IN 3D —

navigation

- [Main Page](#)
- [Table of Contents](#)
- [Structure Index](#)
- [Random](#)
- [Recent Changes](#)
- [Help](#)

search

toolbox

- [Export this page](#)
- [What links here](#)
- [Related changes](#)
- [Upload file](#)
- [Special pages](#)
- [Printable version](#)
- [Permanent link](#)

[Joel L. Sussman](#) [my talk](#) [my preferences](#) [my watchlist](#) [my contributions](#) [log out](#)

[article](#) [discussion](#) [edit this page](#) [history](#) [protect](#) [delete](#) [move](#) [watch](#)

1 open e-mail-confirmed [account request](#) pending

Sandbox 780

Your Heading Here (maybe something like 'Structure') [\[edit\]](#)

This is a default text for your page **Sandbox 780**. Click above on **edit this page** to modify. Be careful with the < and > signs.

You may include any references to papers as in: the use of JSmol in Proteopedia ^[1] or to the article describing Jmol ^[2] to the rescue.

Introduction

Green fluorescent protein (**GFP**), originally isolated from the jellyfish *Aequorea victoria* (PDB entry [1ema](#)), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement. Exploring the Structure

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[toggle spin](#) [toggle quality](#) [popup](#)

Caption for this structure

References

[\[edit\]](#)

HOW TO EDIT A PAGE (7)

Hands-on:

1. We'd now like to add a 3D structure to the page (by adding a Jmol applet displaying the 3D structure for PDB entry 1ema, the structure of Green Fluorescent Protein).
2. In your assigned Sandbox page click on "edit this page".
3. In the text-editing area, change the text at the top
 1. from: load='1stp' to load='1ema' .
 2. from: caption='Caption for this structure' to caption='GFP (PDB entry [[1ema]])'
4. To make things cleaner, delete text: "This is a default text for your page "Sandbox 780". Click above on "edit this page" to modify. Be careful with the < and > signs. You may include any references to papers as in: the use of JSmol in Proteopedia <ref>DOI 10.1002 / ijch.201300024</ref> or to the article describing Jmol <ref>PMID: 21638687</ref> to the rescue."
5. Save the page using the "Save page" button

BOLD AND INTERWIKI LINKS



navigation

- [Main Page](#)
- [Table of Contents](#)
- [Structure Index](#)
- [Random](#)
- [Recent Changes](#)
- [Help](#)

search

toolbox

- [Export this page](#)
- [What links here](#)
- [Related changes](#)
- [Upload file](#)
- [Special pages](#)
- [Printable version](#)
- [Permanent link](#)

Joel L. Sussman [my talk](#) [my preferences](#) [my watchlist](#) [my contributions](#) [log out](#)

[article](#) [discussion](#) [edit this page](#) [history](#) [protect](#) [delete](#) [move](#) [watch](#)

1 open e-mail-confirmed [account request](#) pending

Sandbox 780

Your Heading Here (maybe something like 'Structure') [\[edit\]](#)

Introduction

Green fluorescent protein (**GFP**), originally isolated from the jellyfish *Aequorea victoria* (PDB entry [1ema](#)), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement. Exploring the Structure

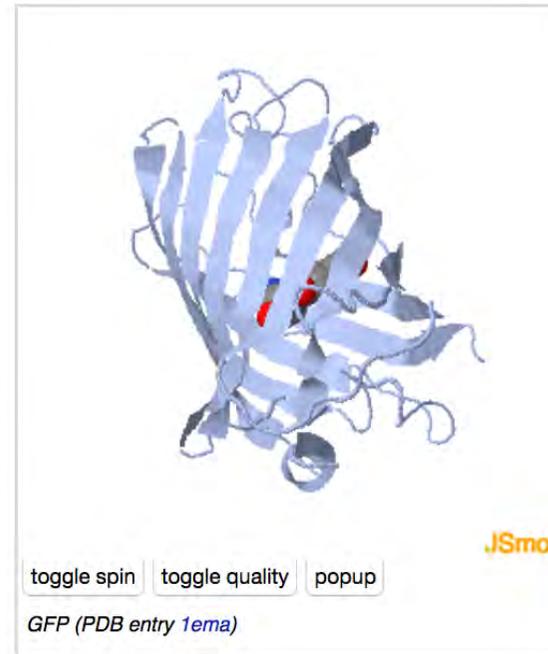
Exploring the Structure

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The chromophore, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of three residues in the central alpha helix: -Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation creates the chromophore's five-membered ring via a new bond between the threonine and the glycine residues.[1]

This is a sample scene created with SAT to [color](#) by Group, and another to make a

References

[\[edit\]](#)



ADDING A GREEN SCENE LINK (1)

Hands-on:

1. Now that we have a 3D model on the page, let's create a **green scene link** that shows 1ema as it looks in the the left part of the 2D image on the GFP Sample page where we got our text. (go back to that page to see what the picture looks like: ([http://proteopedia.org/wiki/index.php/User:Joel L. Sussman/GFP Test Page](http://proteopedia.org/wiki/index.php/User:Joel_L._Sussman/GFP_Test_Page)))
2. To create a green scene link, we will need to use the *Protopedia Scene Authoring Tools*.
3. In your assigned Sandbox page, click on "edit this page".
4. Scroll down to the bold text that says "Scene authoring tools [**show**]" next to a colorful molecule. Click on "**show**" to expand the Scene Authoring Tools.
5. Click on the tab "load molecule" in the Scene Authoring Tools.
6. Load the PDB file 1ema by entering the PDB code "1ema" in the input box next to the words "By PDB code:" and then pressing the adjacent button marked "load".

Your page
should now
look like this:



SAT (Scene Authoring Tools) [\[hide\]](#)

how to load scene save scene

load molecule selections

representations colors labels

Reset

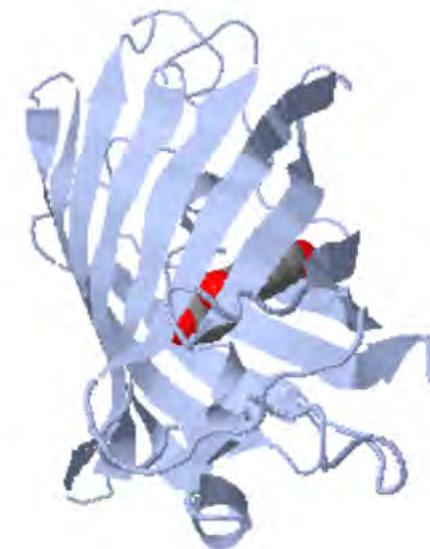
load molecule

By PDB code:

From Proteopedia uploaded file:

*(To load from an uploaded file, first **upload** the file to Proteopedia)*

Add both hydrogens and multiple bonding while loading the structure.



JSmol

currently loaded file	source	timestamp
1ema	PDB	20090520

Select Atoms ALL NONE

Show Selected with Halos ON OFF

<-Undo Redo->

Use Simplified Rendering While Moving

To enable buttons below, save your scene, if desired, then hide the Scene Authoring Tools.

Summary:

ADDING A GREEN SCENE LINK (2)

Hands-on:

1. Now we have 1ema loaded into the Scene Authoring Tools' Jmol applet. The idea behind the Scene Authoring Tools (SAT) is to create the exact scene that you would like to have load when your **green link** is clicked. This is generally done by first loading a PDB file into the SAT's applet, then using the "selections", "representations", "colors", and "labels" tabs to manipulate the 3D model into the desired state, finally saving the **green scene link** using the "save scene" tab.
2. Our structure is currently displayed in cartoon representation. The first step in recreating the picture in the *Molecule of the Month* is to display the molecule in backbone representation.
3. Click on the "selections" tab.
4. In the "all or nothing and halos" section, click on the "select all" button.
5. Nothing changed because "selection halos" were not on. Turn them on by marking the checkbox next to the word "selection halos".
6. Selection halos serve to show you what is currently selected. They will not be displayed when the **green scene link** you eventually create is clicked.

Your page should now look like this:



SAT (Scene Authoring Tools) [\[hide\]](#)

how to load scene save scene load molecule selections

representations colors labels **Reset**

build your selection

groups:

- all
- protein**
- all protein
- alpha carbon
- backbone/mainchain
- helix
- sheet
- sidechain
- turn
- non-protein**

Hold ctrl to select multiple groups

replace selection add to selection remove from selection

limit to chains: limit to residue types:
e.g. A,C,D e.g. PHE,ALA,GLY

sites:

limit to residue numbers:
e.g. 18,23-25,32

limit to elements:
e.g. Fe,2H,31P

invert and center

invert current selection center on current selection

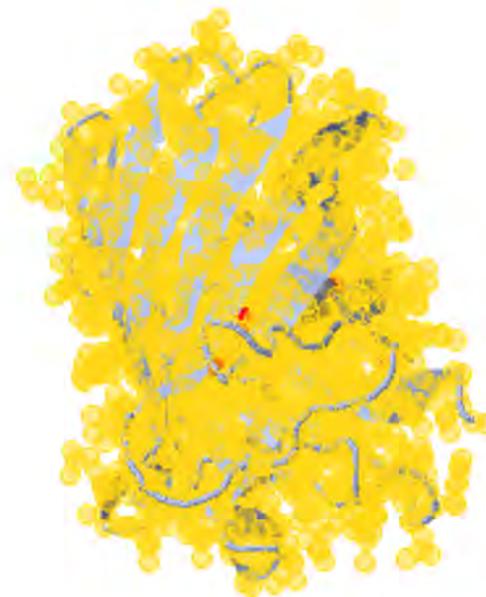
select within distance

Select atoms within Å of current selection.

Expand selection to include entire residues containing any selected atoms.

mouse click selects

nothing center atom element residue/ligand chain



JSmol

currently loaded file	source	timestamp
1ema	PDB	20090520

Select Atoms ALL NONE

Show Selected with Halos ON OFF

Use Simplified Rendering While Moving

ADDING A GREEN SCENE LINK (3)

Hands-on:

1. Now that we have everything selected, click on the “representations” tab of the SAT.
2. Mark the checkbox next to “backbone” in the section titled “set selection representation”.
3. Click on the “set representation” button.
4. Notice the representation of the 3D model has changed from cartoon to backbone. To help see this better, turn off the selection halos by unmarking the checkbox next to “selection halos”.

Your page should now look like this:



SAT (Scene Authoring Tools) [hide]

how to load scene save scene load molecule selections

representations colors labels **Reset**

set selection representation

ball and stick stick/wireframe 90 spacefill 100% dots 100%

backbone 90 trace 90 ribbon cartoon

strands rocket meshribbon 2.5 surface halos

Leaving the input field to the right of a representation-type blank chooses its default setting.
Ball and stick is a combination of wireframe and spacefill.

set representation

hide selection

disulfide and hydrogen bonds [show]



JSmol

currently loaded file	source	timestamp
1ema	PDB	20090520

Select Atoms ALL NONE

Show Selected with Halos ON OFF

<-Undo Redo->

Use Simplified Rendering While Moving

To enable buttons below, save your scene, if desired, then hide the Scene Authoring Tools.

Summary:

ADDING A GREEN SCENE LINK (4)

Hands-on:

1. Now we want to select the segment of the protein that runs through the barrel and color it green.
2. To make a selection, click on the “selections” tab.
3. We will select the segment that runs through the barrel by its residue numbers. To do this we need to know the first and the last residue numbers that make up this segment.
4. Notice that when you hover with your mouse over an atom in the Jmol applet, information about that atom is displayed, including the residue that atom is part of, and the residue number. Use this “hover” feature to find the residue numbers for the beginning and the end of the segment we are interested in.
5. Enter the starting and ending residue numbers, separated by a hyphen, into the input box under the text “limit to residue numbers:”.

Your page should now look like this:



SAT (Scene Authoring Tools) [hide]

how to load scene save scene load molecule selections

representations colors labels **Reset**

build your selection

groups:

- all
- protein**
- all protein
- alpha carbon
- backbone/mainchain
- helix
- sheet
- sidechain
- turn
- non-protein**

Hold ctrl to select multiple groups

replace selection add to selection remove from selection

limit to chains: all limit to residue types: all
e.g. A,C,D e.g. PHE,ALA,GLY

sites: all atoms limit to residue numbers: 54-76
CRO e.g. 18,23-25,32

limit to elements: all
e.g. Fe,2H,31P

invert and center

invert current selection center on current selection

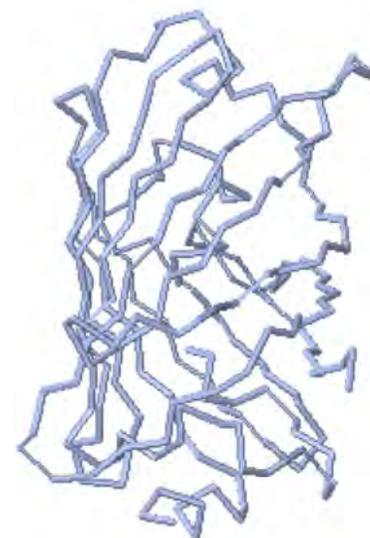
select within distance

Select atoms within Å of current selection.

Expand selection to include entire residues containing any selected atoms.

mouse click selects

nothing center atom element residue/ligand chain



JSmol

currently loaded file	source	timestamp
1ema	PDB	20090520

Select Atoms ALL NONE

Show Selected with Halos ON OFF

<-Undo Redo->

Use Simplified Rendering While Moving

ADDING A GREEN SCENE LINK (5)

Hands-on:

1. Having entered the starting and ending residue numbers of the chain segment into the “limit by residue numbers” input box, we are ready to make a selection that is limited only to the stretch of residues that we desire.
2. Before making our new selection, let’s turn on selection halos so we see the change in the selection take place. Mark the checkbox next to “selection halos”. Notice that everything is selected.
3. Now go ahead and make the new selection by clicking “replace selection”. This will replace the old selection (everything) with our new selection (limited to a stretch of residues).

Your page should now look like this:



SAT (Scene Authoring Tools) [hide]

how to load scene save scene load molecule selections

representations colors labels **Reset**

build your selection

groups:

- all
- protein**
- all protein
- alpha carbon
- backbone/mainchain
- helix
- sheet
- sidechain
- turn
- non-protein**

Hold ctrl to select multiple groups

replace selection add to selection remove from selection

limit to chains: all limit to residue types: all
e.g. A,C,D e.g. PHE,ALA,GLY

sites: all atoms limit to residue numbers: 54-76
CRO e.g. 18,23-25,32

limit to elements: all
e.g. Fe,2H,31P

invert and center

invert current selection center on current selection

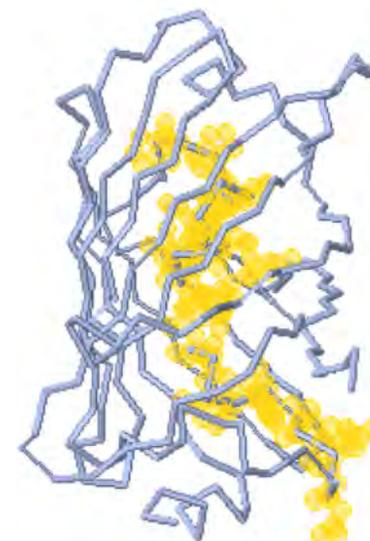
select within distance

Select atoms within Å of current selection.

Expand selection to include entire residues containing any selected atoms.

mouse click selects

nothing center atom element residue/ligand chain



JSmol

currently loaded file	source	timestamp
1ema	PDB	20090520

Select Atoms ALL NONE

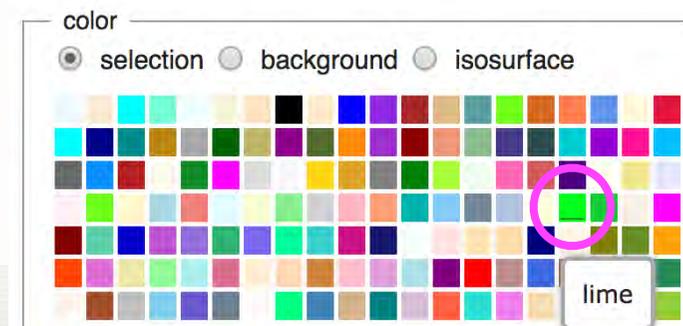
Show Selected with Halos ON OFF

▾

ADDING A GREEN SCENE LINK (6)

Hands-on:

1. With the chain segment selected, it's time to change its color to match the image in the Molecule of the Month.
2. Click on the "colors" tab of the Scene Authoring Tools.
3. Click on a lime color in the color palette to change the color of the selected chain segment. Turn off selection halos to better view the change in color.
4. Now let's make the background black.
5. In the section titled "color", mark the button next to "background". Now any color you select from the color palette will affect the background instead of the selection.
6. Click on the color black in the color palette.



Your page should now look like this:



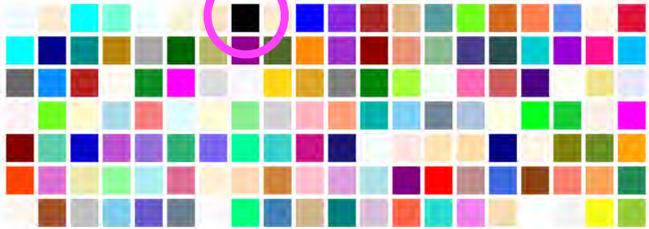
SAT (Scene Authoring Tools) [hide]

how to load scene save scene load molecule selections

representations colors labels **Reset**

color

selection background isosurface



elements (CPK) composition chain

N->C rainbow (named chain) N->C rainbow (polymer)

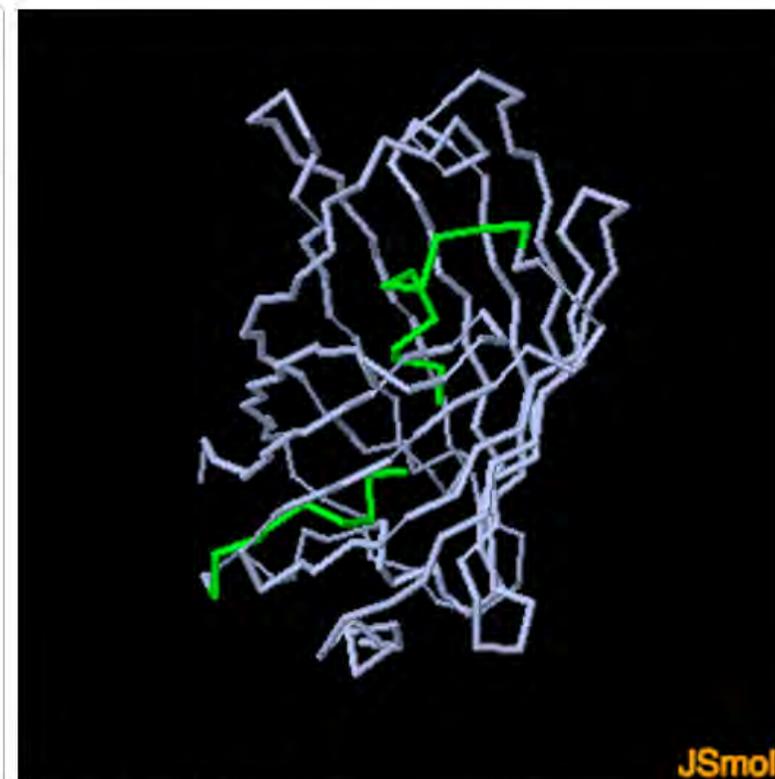
secondary structure hydrophobic/polar

charge, protein evolutionary conservation

temperature, fixed temperature, relative

transparency

0 % transparent go



currently loaded file	source	timestamp
1ema	PDB	20090520

Select Atoms ALL NONE

Show Selected with Halos ON OFF

<-Undo Redo->

Use Simplified Rendering While Moving ▾

ADDING A GREEN SCENE LINK (7)

Hands-on:

1. All that's left is to show the chromophore and color it in the CPK scheme.
2. Click on the "selections" tab.
3. In the input box under "limit to residue types:" type "CRO". (In the PDB file, the chromophore is listed as a residue with type "CRO")
4. Click on the "replace selection" button. Turn on selection halos.
5. Click on the "representations" tab.
6. In the section titled "set selection representation" mark the checkbox next to stick/wireframe. Click on the "set representation" button.
7. Click on the "colors" tab.
8. In the section titled "color" click on the button titled "CPK (by element)".
9. Turn off selection halos to better view the new color.

Your page should now look like this:



SAT (Scene Authoring Tools) [hide]

how to | load scene | save scene | load molecule | selections

representations | colors | labels | **Reset**

color

selection background isosurface



elements (CPK) | composition | chain

N->C rainbow (named chain) | N->C rainbow (polymer)

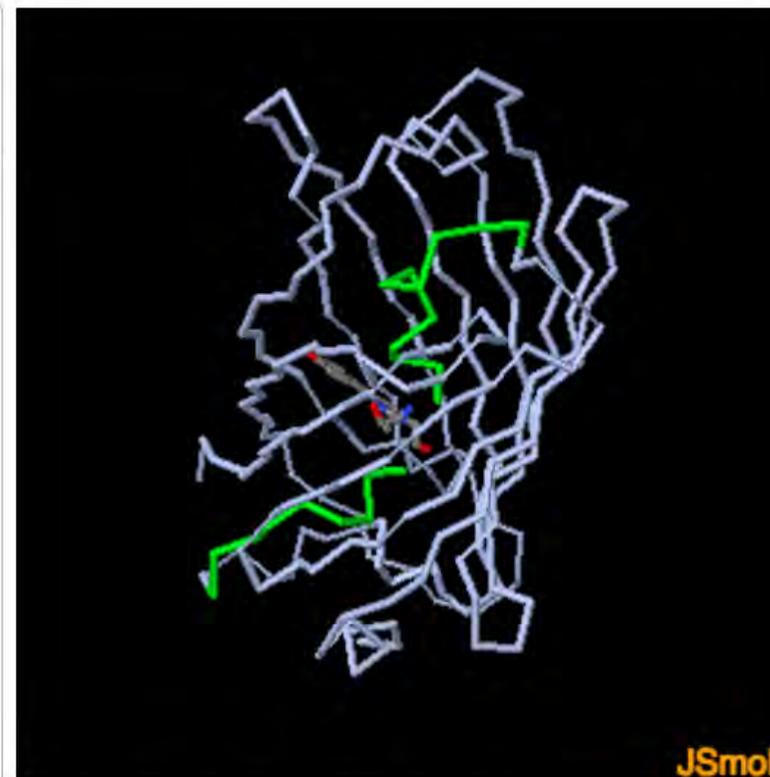
secondary structure | hydrophobic/polar

charge, protein | evolutionary conservation

temperature, fixed | temperature, relative

transparency

0 % transparent go



currently loaded file	source	timestamp
1ema	PDB	20090520

Select Atoms ALL NONE

Show Selected with Halos ON OFF

<-Undo Redo->

Use Simplified Rendering While Moving ▾

ADDING A GREEN SCENE LINK (8)

Hands-on:

1. Notice that connection between the chromophore & the chain is missing, but is seen in the original picture: [http://proteopedia.org/wiki/index.php/User:Joel L. Sussman/GFP Test Page](http://proteopedia.org/wiki/index.php/User:Joel_L._Sussman/GFP_Test_Page). Let's visualize those missing bonds in the chain.
2. Click on the "selections" tab; in the 'build your selection' box, under 'groups' select 'backbone/mainchain'; In the input box under "limit to residue numbers:" type "64,68". (These are the numbers of the residues directly preceding and following the chromophore.)
3. Click on the "add to selection" button.
4. Click on the "representations" tab.
5. In the section titled "set selection representation" mark the checkbox next to stick/wireframe. Click on the "set representation" button.
6. Click on the "colors" tab.
7. In the section titled "color" click on the button titled "CPK (by element)".
8. Turn off selection halos to better view the new color.

ADDING A GREEN SCENE LINK (9)

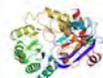
Hands-on:

1. Our scene is done, so let's save it and put it into the page.
2. Click on the "save scene" tab in the Scene Authoring Tools.
3. Give your scene a name and a description by entering text in the "Name" and "Description" text-areas.
4. Let's make our scene spin when it loads. In the drop down menu next to the text "when this scene loads, I want it to" choose the option "spin".
5. Click on the "save scene" button.

Your page should now look like this:

Please note that all contributions to Proteopedia may be edited, altered, or removed by other contributors. If you don't want your writing to be edited mercilessly, then don't submit it here.

You are also promising us that you wrote this yourself, or copied it from a public domain or similar free resource (see [Project:Copyrights](#) for details). **DO NOT SUBMIT COPYRIGHTED WORK WITHOUT PERMISSION!**



SAT (Scene Authoring Tools) [\[hide\]](#)

how to | load scene | save scene | load molecule | selections

representations | colors | labels | **Reset**

Save current scene

Scene name

e.g. Active_site_gorge
Enter an existing scene name to save as the most recent version (will not overwrite).

Scene description (recomended)

when this scene loads, I want it to

Use Default Rendering While Rotating

Always Reload Structure When Loading this Scene

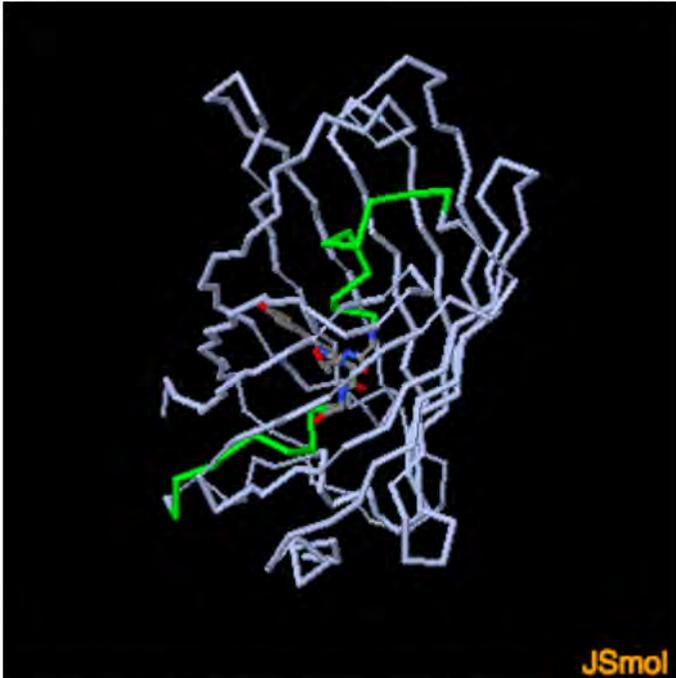
show scene transition options?

Wikitext

Copy and paste the following line where you want the scene link to appear (scroll down if needed) and edit the TextToBeDisplayed:

```
<scene name='61/612803/1ema_chromophore/1'>TextToBeDisplayed</scene>
```

Upon saving a scene, wikitext for creating a link to the saved scene will appear above.



currently loaded file	source	timestamp
1ema	PDB	20090520

Select Atoms ALL NONE

Show Selected with Halos ON OFF

Use Simplified Rendering While Moving

ADDING A GREEN SCENE LINK (9)

Hands-on:

1. As soon as we saved our scene, some wikitext appeared in the text-area titled “Wikitext” that was previously empty.
2. The new text in the “Wikitext” text-area instructs you to copy a line in the text-area & paste it in the text of the Proteopedia page where you would like the **green scene link** to appear. The line looks similar to this: `<scene name='61/612803/1ema_chromophore/1'>TextToBeDisplayed</scene>>`
3. Highlight that line in the “Wikitext” text-area and copy it.
4. Scroll up the page, past the Scene Authoring Tools to the text-editing area of the Proteopedia page.
5. Find the word “chromophore” in the text-editing area. Highlight it and replace it by pasting the text you previously copied in step (3).

Your page should now look like this:

Editing Sandbox 780



==Your Heading Here (maybe something like 'Structure')==

<StructureSection load='1ema' size='340' side='right' caption='GFP (PDB entry [[1ema]])' scene=''>

== Introduction ==

Green fluorescent protein ("GFP"), originally isolated from the jellyfish *Aequorea victoria* (PDB entry [[1ema]]), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement.

Exploring the Structure

== Exploring the Structure ==

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The <scene name='61/612803/1ema_chromophore/1'>TextToBeDisplayed</scene>, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of three residues in the central alpha helix: -Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation creates the chromophore's five-membered ring via a new bond between the threonine and the glycine residues.[1]

ADDING A GREEN SCENE LINK (10)

Hands-on:

1. The text that you just pasted from the “Wikitext” section of the Scene Authoring Tools creates a **green scene link** wherever you place it in the Proteopedia page.
2. The word “**TextToBeDisplayed**” will be the part that shows up as the text of the green link on the page.
3. Change “**TextToBeDisplayed**” to say “**chromophore**”. It should look something like:

```
<scene name='Sandbox_780/1ema_chromophore/1'>chromophore</scene>
```
4. Scroll down to the bold text “Scene Authoring Tools [**hide**]” next to the colored molecule, and click on “**hide**” to hide the Scene Authoring Tools.
5. Scroll down and click on “Save page” to save the Proteopedia page you edited.
6. Try clicking on the new **green scene link** you have created.

Your page
should
now look
like this:

[article](#) [discussion](#) [edit this page](#) [history](#) [protect](#) [delete](#) [move](#) [watch](#)

1 open e-mail-confirmed [account request](#) pending

Sandbox 780

Your Heading Here (maybe something like 'Structure') [\[edit\]](#)

Introduction

Green fluorescent protein (**GFP**), originally isolated from the jellyfish *Aequorea victoria* (PDB entry [1ema](#)), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement.

Exploring the Structure

Exploring the Structure

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The **chromophore**, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing



JSmol

[toggle spin](#) [toggle quality](#) [popup](#)

GFP (PDB entry [1ema](#))

ADDING A 'HEADING'

Hands-on:

1. To make the page look nicer, need add a 'Heading' to first paragraph.
2. Go back and Edit your page
3. Change, in the top line of your text
 - ==Your Heading Here (maybe something like 'Structure')==<StructureSection. . .
 - to
 - == **Example page for Green fluorescent protein ("GFP")** ==<StructureSection. . .
4. Save page

Your page
should
now look
like this:

[article](#) [discussion](#) [edit this page](#) [history](#) [protect](#) [delete](#) [move](#) [watch](#)

1 open e-mail-confirmed [account request](#) pending

Sandbox 780

Example page for Green fluorescent protein (**GFP**) [\[edit\]](#)

Introduction

Green fluorescent protein (**GFP**), originally isolated from the jellyfish *Aequorea victoria* (PDB entry [1ema](#)), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement.

Exploring the Structure

Exploring the Structure

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The **chromophore**, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing



[toggle spin](#) [toggle quality](#) [popup](#) **JSmol**

GFP (PDB entry [1ema](#))

ADDING A REFERENCE

Hands-on:

1. Let's cite a reference in our page. Look at the reference at the bottom of our original example page: [http://proteopedia.org/wiki/index.php/User:Joel L. Sussman/GFP Test Page](http://proteopedia.org/wiki/index.php/User:Joel_L._Sussman/GFP_Test_Page).
2. We *could* add the reference by typing it out -- that's the long way.
3. A much easier way is to refer to the paper by its PubMed ID: Click on 'edit this page' for your 'Sandbox' page. At the end of the 2nd paragraph, after the words 'the glycine residues', add the text '`<ref>PMID:8703075</ref>`'.
4. '`<ref>`' is called the opening reference tag, and '`</ref>`' is the closing tag. Together they enclose the text 'PMID:' which stands for PubMed ID, and then the actual PubMed ID of the reference you want to cite.
5. You've added the citation, but you still need to specify where the bibliography will appear -- the list of all cited references in the page. This was automatically added when you created your page, *i.e.* the line '`<references/>`' after the last paragraph.
6. To simplify, **delete** text "This is a sample scene created with SAT. . . of these sample scenes."
7. Save the page.

Editing Sandbox 780



```
== Example page for Green fluorescent protein ("GFP") ==  
<StructureSection load='1ema' size='340' side='right' caption='GFP (PDB entry [[1ema]])' scene=''>
```

```
== Introduction ==
```

Green fluorescent protein ("GFP"), originally isolated from the jellyfish *Aequorea victoria* (PDB entry [[1ema]]), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement.

Exploring the Structure

```
== Exploring the Structure ==
```

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The `<scene name='61/612803/1ema_chromophore/1'>chromophore</scene>`, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of three residues in the central alpha helix: -Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation creates the chromophore's five-membered ring via a new bond between the threonine and the glycine residue: `<ret>PMID:8703075</ret>`.

```
</StructureSection>
```

```
== References ==
```

```
<references/>
```

Your page
should
now look
like this:

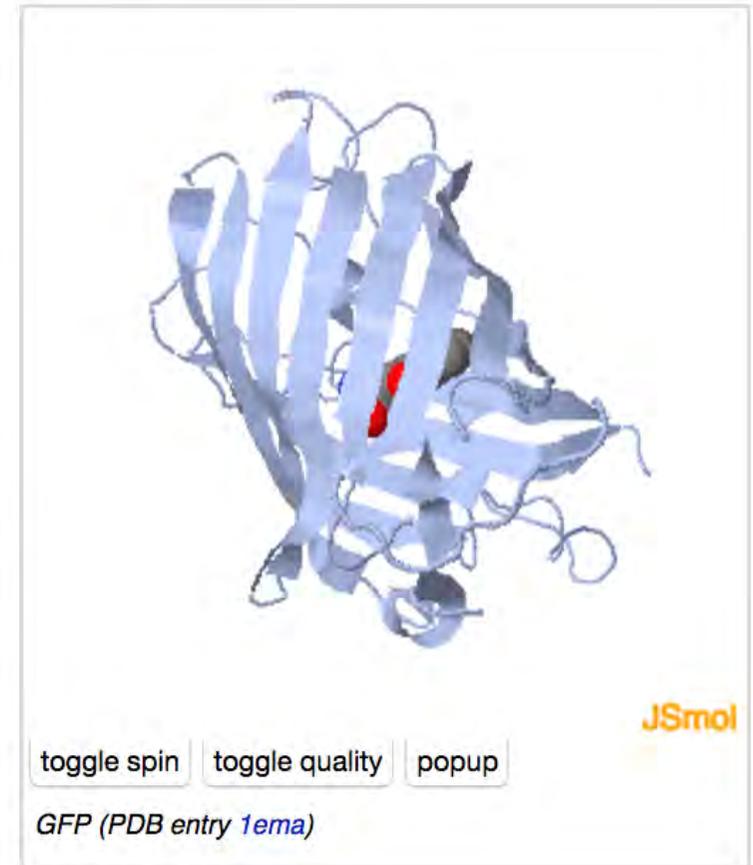
Example page for Green fluorescent protein (GFP) [\[edit\]](#)

Introduction

Green fluorescent protein (**GFP**), originally isolated from the jellyfish *Aequorea victoria* (PDB entry [1ema](#)), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement. Exploring the Structure

Exploring the Structure

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The **chromophore**, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of three residues in the central alpha helix: -Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation creates the chromophore's five-membered ring via a new bond between the threonine and the glycine residues^[1].

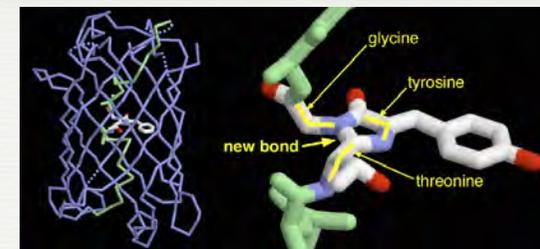


References [\[edit\]](#)

1. ↑ Ormo M, Cubitt AB, Kallio K, Gross LA, Tsien RY, Remington SJ. Crystal structure of the *Aequorea victoria* green fluorescent protein. *Science*. 1996 Sep 6;273(5280):1392-5. PMID:[8703075](#) [↗](#)

ADDING A 2D IMAGE (1)

Hands-on:



- Let's add a 2D image to our page. View our example page [http://proteopedia.org/wiki/index.php/User:Joel L. Sussman/GFP Test Page](http://proteopedia.org/wiki/index.php/User:Joel_L._Sussman/GFP_Test_Page) and save the big picture to your computer by right-clicking on it and choosing an option like "Save as..." or "Save to desktop". Save the image (1ema.gif) to your desktop.
- We now need to upload the image to Proteopedia. Back in your Proteopedia 'Sandbox' page, click on the '[upload file](#)' link in the left-hand toolbar

search

Go Search

toolbox

- [Export this page](#)
- [What links here](#)
- [Related changes](#)
- [Upload file](#)
- [Special pages](#)
- [Printable version](#)
- [Permanent link](#)

ADDING A 2D IMAGE (2)

Hands-on:

1. At the 'upload file' page, next to 'Source filename:' click on the 'Choose file' button. Using the interface that pops up, browse to and select the 2D image we saved (1ema.gif). **Choose File**
2. On the 'upload file' page, make sure to change the 'Destination filename' from '1ema.gif' to something unique like '1ema_Workshop_579.gif' where 'Workshop' is the name of your workshop, and '579' is your 'Sandbox' number.
3. Under 'Summary' type a short summary of what we see in the picture 1ema.gif.
4. Click on the 'Upload file' button. **Upload file**
5. Your file will be uploaded and you will be taken to it's new page in Proteopedia.
6. Copy the image's name, so you have it for later:



ADDING A 2D IMAGE (3)

Hands-on:

1. Go back to your 'Sandbox' page and click on 'edit this page'.
2. Click on the text-editing area just before text "Green fluorescent protein . . ." and hit carriage return to add one blank line.
3. Click so that your cursor is in the white space you just created.
4. Now click on the button that looks like a picture. This will insert wiki-text for a 2D image.

Editing Sandbox 780



```
== Example page for Green fluorescent protein ("GFP") ==  
<StructureSection load='1ema' size='340' side='right' caption=  
scene="">
```

| <--- **Cursor here**

```
== Introduction ==
```

Green fluorescent protein ("GFP"), originally isolated from the entry [[1ema]], fluoresces green (509nm) when exposed to blue

ADDING A 2D IMAGE (4)

Hands-on:

1. After you clicked on the button that looks like a picture, some wiki-text should have popped up that says '`[[Image:Example.jpg]]`'.
2. Note that this format of double square brackets is the same format as for internal links that we created earlier to '1ema' (`[[1ema]]`).
3. Change the word 'Example.jpg' to the name of your image (remember, you copied the name of your image before, now it comes in handy, you may paste it.)
4. The final result should look something like this '`[[Image:1ema_Workshop_579.jpg]]`'
5. Save the page.

Editing Sandbox 780



```
== Example page for Green fluorescent protein ("GFP") ==  
<StructureSection load='1ema' size='340' side='right' caption  
scene=''>  
[[Image:1ema.gif]]  
== Introduction ==
```

ADDING A 2D IMAGE (5)

Hands-on:

1. At this point you should see the 2D image on your page, but it should be huge -- way too big for us. Let's change that -- click on 'edit this page'
2. Change '`[[Image:1ema.gif]]`' by adding additional parameters, each separated by a vertical bar '|'.
3. You should change it to read:
'`[[Image:1ema.gif|thumb|left|350px|Green fluorescent protein (1ema)]]`'
4. This specifies that the image should be a thumbnail on the left side of the page of size 350 pixels and with the caption 'Green fluorescent protein (1ema)'.
5. Save the page.



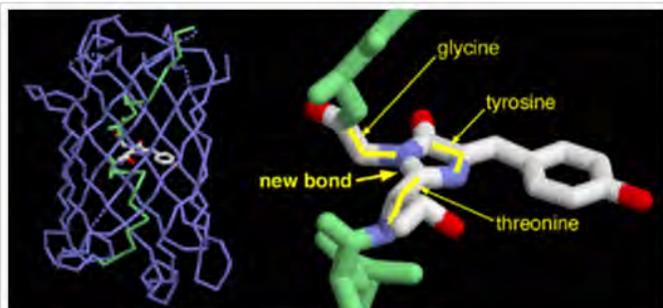
```
== Example page for Green fluorescent protein ("GFP") ==  
<StructureSection load='1ema' size='340' side='right' caption='GFP (PDB entry [[1ema]])'  
scene="">  
[[Image:1ema.gif|thumb|left|350px|Green fluorescent protein (1ema)]]  
== Introduction ==
```

Your page should now look like this:

Sandbox 780

Example page for Green fluorescent protein (**GFP**)

[edit]



Green fluorescent protein (1ema)

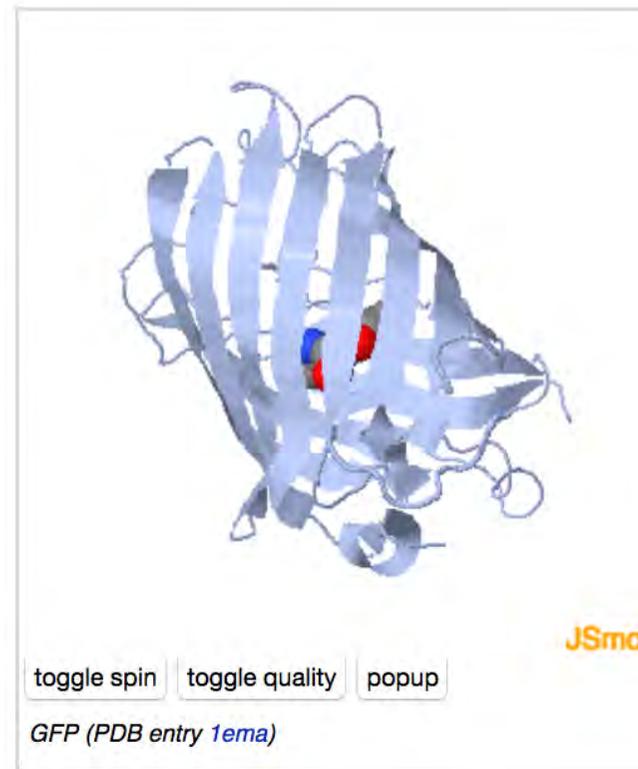
Introduction

Green fluorescent protein (**GFP**), originally isolated from the jellyfish *Aequorea victoria* (PDB entry [1ema](#)), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological

research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement. Exploring the Structure

Exploring the Structure

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The **chromophore**, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of three residues in the central alpha helix: - Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation creates the chromophore's five-membered ring via a new bond between the threonine and the glycine residues^[1].



toggle spin toggle quality popup

GFP (PDB entry [1ema](#))

[edit]

References

1. ↑ Ormo M, Cubitt AB, Kallio K, Gross LA, Tsien RY, Remington SJ. Crystal structure of the *Aequorea victoria* green fluorescent protein. *Science*. 1996 Sep 6;273(5280):1392-5. PMID:[8703075](#)

ADDING A QUIZ

Hands-on:

1. We want to add a quiz to the page to test the reader's comprehension. Click on 'edit this page'.
2. Add the following text after the line '<references/>'
3. '==Quiz==' is a section heading as before. The rest is wiki-text for a quiz. Save page.

The question is between two curly brackets. Each potential answer is on its own line. A wrong answer is preceded by a minus ('-') sign and the correct answer by the plus ('+') sign.

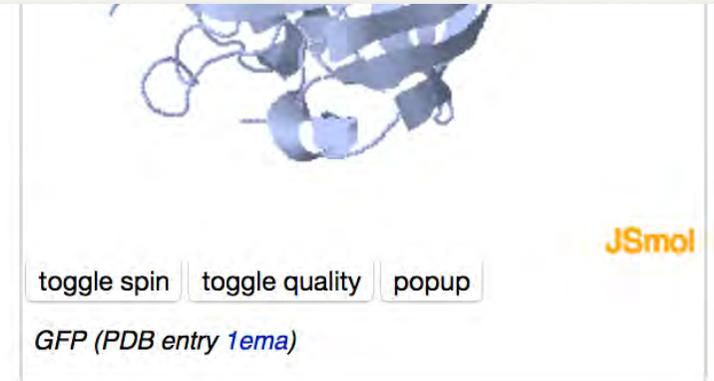
```
<references/>

==Quiz==
<quiz display=simple>
{How many alpha helices are in this structure?}
- One
- None
+ Eleven
- Twelve
</Quiz>
```

Your page
should
now look
like this:

Exploring the Structure

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The **chromophore**, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of three residues in the central alpha helix: -Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation creates the chromophore's five-membered ring via a new bond between the threonine and the glycine residues^[1].



References

[edit]

1. ↑ Ormo M, Cubitt AB, Kallio K, Gross LA, Tsien RY, Remington SJ. Crystal structure of the Aequorea victoria green fluorescent protein. Science. 1996 Sep 6;273(5280):1392-5. PMID:8703075 [↗](#)

Quiz

[edit]

1. How many alpha helices are in this structure?
 - One
 - None
 - Eleven
 - Twelve

Submit

-Try taking your quiz by selecting an answer and clicking on the 'Submit' button.-

YOUR OWN ACCOUNT

- If you want to use Proteopedia in the future to create your own pages, please request your own account in your own name. You can do this now if you want!
- Request an account in your name by logging out of guest account and clicking “log in / request account” at top right corner of website. Enter the information that is requested, and your account will be approved by Prof. Eric Martz (Univ of Mass).

HELP RESOURCES



- General Help: <http://www.proteopedia.org/w/Help:Contents>
- Editing Help: <http://www.proteopedia.org/w/Help:Editing>
- Wikitext Cheatsheet: <http://en.wikipedia.org/wiki/Wikipedia:Cheatsheet>
- Scene Authoring Tools Help: http://www.proteopedia.org/w/Scene_authoring_tools
- Proteopedia Video Guide: http://www.proteopedia.org/w/Proteopedia:Video_Guide

- Lac Repressor :
http://www.proteopedia.org/w/Lac_repressor
- 2q66 - Poly(A) polymerase :
<http://www.proteopedia.org/w/2q66>
- HIV-1 Protease :
http://www.proteopedia.org/w/HIV-1_protease
- Avian Influenza Neuraminidase, Tamiflu and Relenza :
http://www.proteopedia.org/w/Avian_Influenza,_Tamiflu_and_Relenza
- Recoverin: a calcium-activated myristoyl switch :
http://www.proteopedia.org/w/Recoverin,_a_calcium-activated_myristoyl_switch
- **A Physical Model of the β 2-Adrenergic Receptor**
http://proteopedia.org/w/Group:SMART:A_Physical_Model_of_the_beta-2-Adrenergic_Receptor





References:

- Hodis, Prilusky, Martz, Silman, Moult & Sussman (2008) “Proteopedia – a scientific ‘wiki’ bridging the rift between 3D structure and function of biomacromolecules” *Genome Biol* **9**, R121.
- Prilusky, Hodis, Canner, Decatur, Oberholser, Martz, Berchanski, Harel & Sussman (2011) “Proteopedia: A status report on the collaborative, 3D web-encyclopedia of proteins and other biomolecules” *J of Struct Biol* **175**, 244-252.
- Hanson, Prilusky, Renjian, Nakane & Sussman (2013) “JSmol and the Next-Generation Web-Based Representation of 3D Molecular Structure as Applied to Proteopedia” *Israel J of Chem* **53**, 207-216.