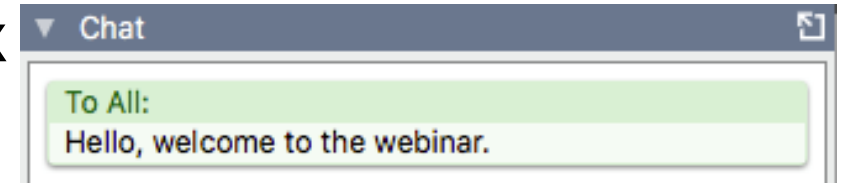


Welcome!

Webinar instructions:

- GoToTraining works best in **Chrome** or on Linux, **Firefox**
- All **microphones will be muted** while the trainer is speaking
- If you have a question, please use the **chat box** at the bottom of the GoToTraining box
- Please complete the **feedback survey** which will launch at the end of the webinar



PDBe API webinar series:

6th Webinar

Data Visualisation at PDBe



Mandar Deshpande



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[proteindatabank](https://www.youtube.com/proteindatabank)



[pdbeurope](https://www.instagram.com/pdbeurope)



[pdbart](https://www.pinterest.com/pdbart)

Agenda

1. Fundamentals

Why, Which and How

2. Resources

Documentation, Demos and more

3. Example

PDBe Molstar & ProtVista integration

Fundamentals

Why, Which and How



Why Data Visualisation?

- Easy comprehension of huge/complex data
- Finding correlation between different data
- Facilitate interaction
- Communicate findings
- Cross-linking resources

How we decide?

- **Standard representations**

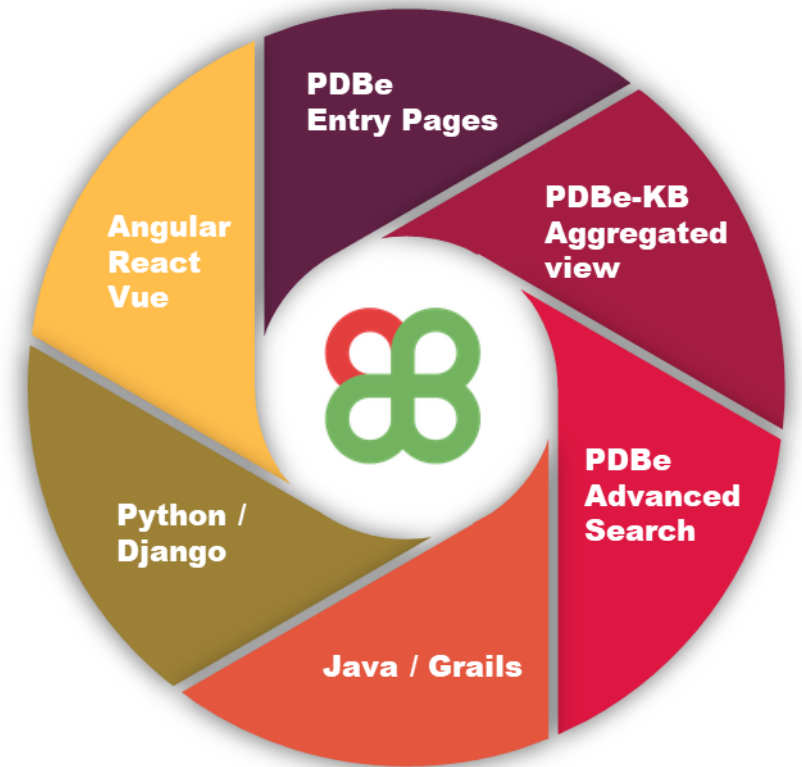
- Icons, Logos, Feature viewers, 2D/3D viewers, etc.

- **UX/UI exercise**

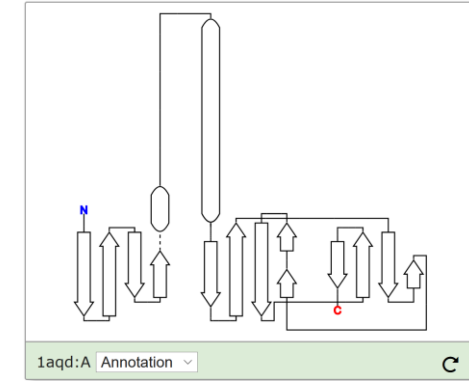
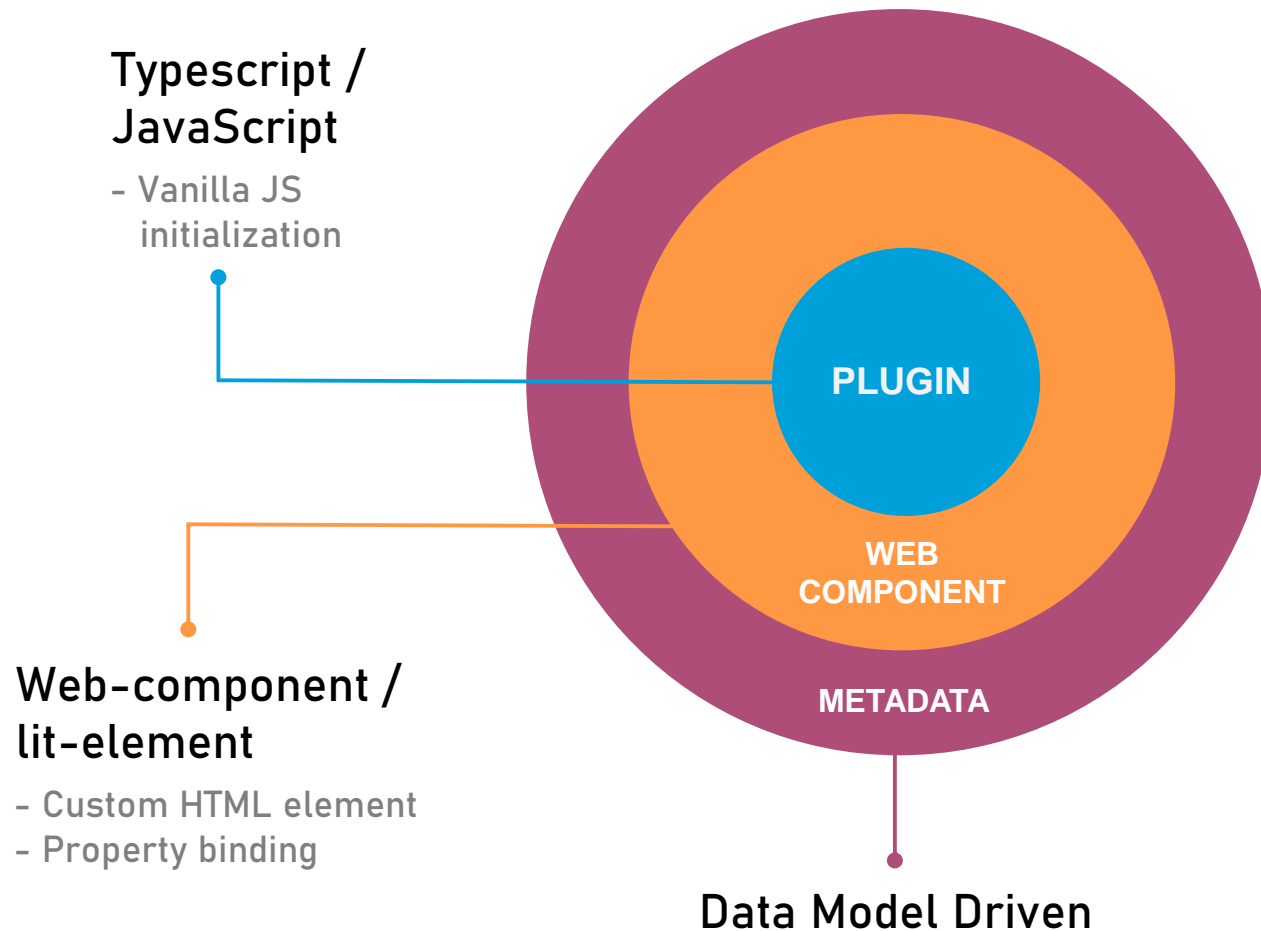
- Identify users (personas)
- Scientific questions which needs to be answered
- Sketching exercise, Wire-frames and Mock-ups
- User testing, feedback and improvement (Iterative)

Visualisation for all!

- Standalone Web components / Plugins
- Framework agonistic
- Distribution
 - PDB Component Library
 - BioJS Library
 - GitHub
 - NPM



Design



PDB Topology Viewer

Plugin

```
const viewerInstance = new PdbTopologyViewerPlugin();  
viewerInstance.render(viewerContainer, options);
```

Web component

```
<pdb-topology-viewer pdb-id="1cbs" entity-id="1"></pdb-topology-viewer>
```


Resources

Documentation, Demos and more...



Data Visualisations



PDB Prints



PDB-REDO

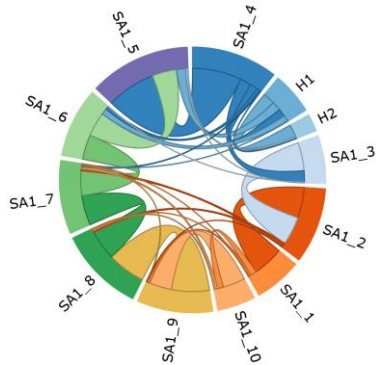
Assembly 1 ●

Confidence : 18%

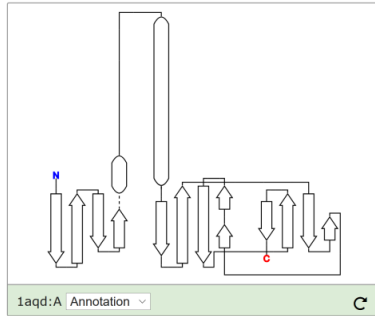
No. subunits : 2

Symmetry : C2 [More details](#)

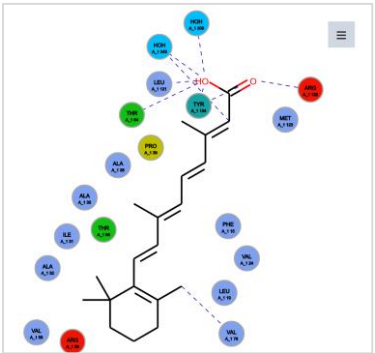
PDB 3D Complex



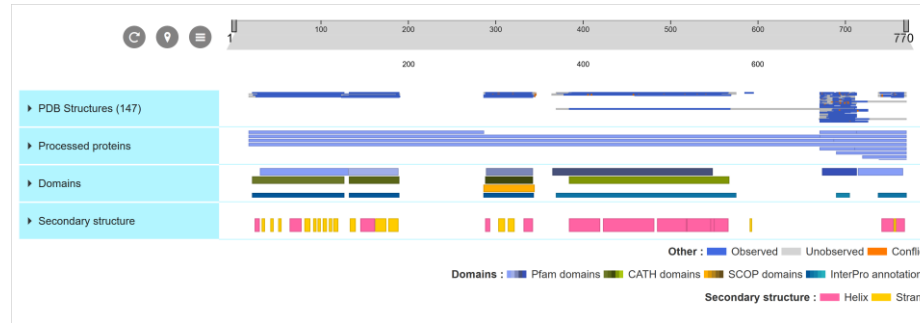
PDB Residue Interactions



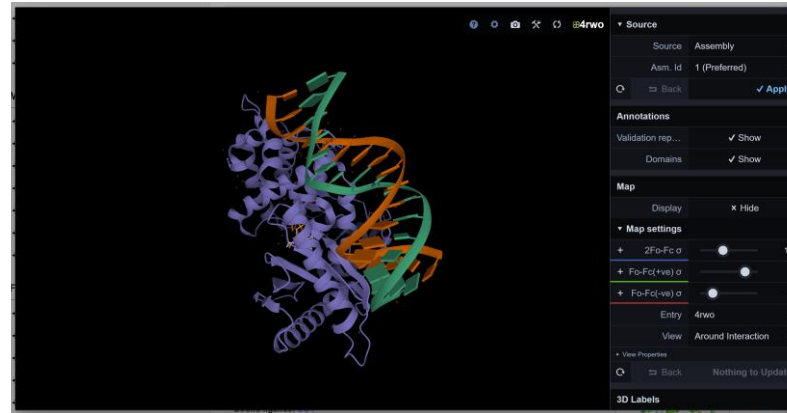
PDB Topology Viewer



PDB Ligand Environment



PDB ProtVista

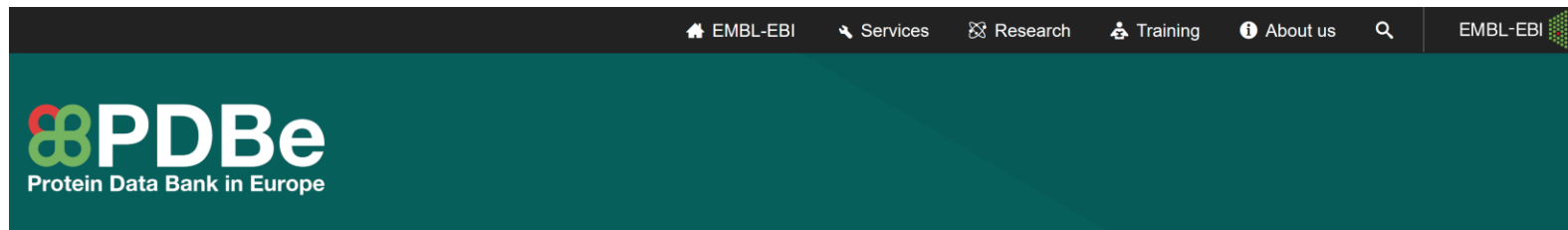


PDBe Molstar

Collaborations



PDB Component Library



PDBE / PDB COMPONENT LIBRARY

PDB Component Library

PDBe Molstar

PDBe Molstar is a streamlined structure viewer which enables a PDB structure to be explored within a browser rather than requiring pre-installed molecular graphics software. Navigation is simple, with rotation of the camera using the left mouse button, zooming controlled with the right mouse button and clicking on a residue or atom to center the view to this point. There is also the option to view electron density of the structure where structure factors have been deposited to the PDB. PDBe Molstar also displays validation and domain information for the structure.

This is a PDBe implementation of [Molstar](#) project.

Collaborations



Resources

Source code: [GitHub](#)

Documentation and working examples: [GitHub Wiki](#)

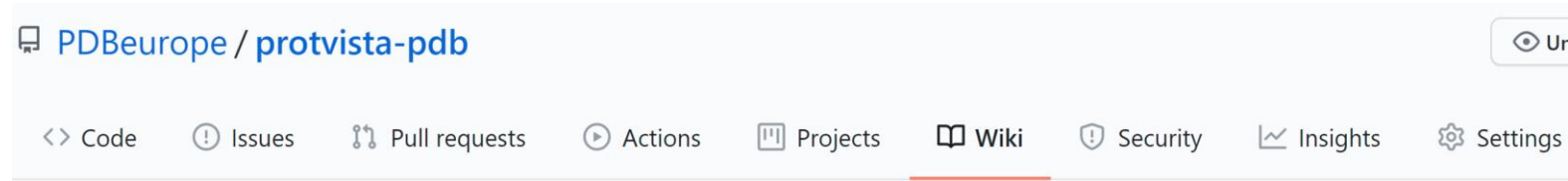
Demo



```
<pdbe-molstar molecule-id="1cbs" hide-controls="true"></pdbe-molstar>
```

Refer [here](#) for details of all the available attributes

Wiki Documentation



Steps to include ProtVista PDB as a web component in a web application

1. Include the style and script files of the library in your web page

```
<!-- CSS -->
<link rel="stylesheet" href="https://ebi.emblstatic.net/web_guidelines/EBI-Icon-fonts/v1.2/fonts.css" type="text/css" media="all"/>

<!-- JS -->
<script src="https://d3js.org/d3.v4.min.js"></script>
<script src="https://www.ebi.ac.uk/pdbe/pdb-component-library/js/protvista-pdb-2.0.0.js"></script>
```

*Until web components are natively supported by all browsers, it is necessary to use polyfills

2. Include ProtVista PDB as HTML Element

```
<protvista-pdb accession="P05067"></protvista-pdb>
```

Working Example

- [ProtVista PDB demo](#)
- [ProtVista PDB custom data demo](#)

Working examples

The image displays a web browser window with a code editor on the left and a preview of a web page on the right. The code editor shows the HTML code for a page titled "ProtVista PDB Demo". The code includes a head section with links to a stylesheet and JavaScript files, and a body section with a heading, an actions menu, and several buttons for zooming, highlighting, and resetting the view.

```
1 <!DOCTYPE html>
2 <html>
3
4 <head>
5
6 <link rel="stylesheet" href="https://ebi.emblstatic.
  net/web_guidelines/EBI-Icon-fonts/v1.2/fonts.css"
  type="text/css" media="all"/>
7 <script src="https://d3js.org/d3.v4.min.js"
  charset="utf-8"></script>
8 <script type="text/javascript" src="https://www.ebi.
  ac.uk/pdbe/pdb-component-library/js/protvista-pdb-2.
  0.0.js"></script>
9
10 </head>
11
12 <body>
13 <h4>ProtVista PDB Demo</h4>
14
15 <!-- Actions Menu -->
16 <div style="float:right; border:1px solid lightgray;
  width:300px;padding:10px;display:none">
17
18 <h3><u>Helper methods</u></h3>
19 <button id="zoomBtn">Zoom on 100-200 range</button>&
  nbsp;
20 <button id="resetZoomBtn">Reset zoom</
  button><br><br>
21 <button id="highlightBtn">Highlight on 133-189
  range</button>&nbsp;nbsp;nbsp;
22 <button id="clearHighlightBtn">Reset Highlight</
  button><br><br>
23 <button id="resetViewBtn">Reset View</
```

The preview window shows the rendered page. It features a navigation bar with a refresh button, a location pin, and a menu icon. Below the navigation bar is a scale bar from 0 to 770. The main content area displays a protein structure visualization with various annotations. The annotations are organized into a list on the left side of the visualization:

- PDB Structures (147)
- Domains
- Secondary structure
- Ligand binding sites
- Interaction interfaces
- Predicted functional sites
- Predicted PTM sites
- Predicted ligand

Red arrows point to the "Fork" and "Download" icons in the browser's top right corner.

<https://github.com/PDBEurope/protvista-pdb/wiki#working-example>

Example

PDBe Molstar & ProtVista integration



Integration – PDBe Molstar

Step 1 : Include visualisation library files in the web application

Files for Plugin implementation

```
<!-- CSS -->  
<link rel="stylesheet" href="https://www.ebi.ac.uk/pdbe/pdb-component-library/css/pdbe-molstar-1.1.0.css">  
  
<!-- JS -->  
<script src="https://www.ebi.ac.uk/pdbe/pdb-component-library/js/pdbe-molstar-plugin-1.1.0.js"></script>
```

Files for Web component implementation

```
<!-- Web component Polyfills -->  
<!-- Required for IE11 -->  
<script src="https://cdn.jsdelivr.net/npm/babel-polyfill/dist/polyfill.min.js"></script>  
<!-- Web component polyfill (only loads what it needs) -->  
<script src="https://cdn.jsdelivr.net/npm/@webcomponents/webcomponentsjs/webcomponents-lite.js" charset="utf-8"></script>  
<!-- Required to polyfill modern browsers as code is ES5 for IE... -->  
<script src="https://cdn.jsdelivr.net/npm/@webcomponents/webcomponentsjs/custom-elements-es5-adapter.js" charset="utf-8"></script>  
  
<!-- CSS -->  
<link rel="stylesheet" href="https://www.ebi.ac.uk/pdbe/pdb-component-library/css/pdbe-molstar-1.1.0.css">  
  
<!-- JS -->  
<script src="https://www.ebi.ac.uk/pdbe/pdb-component-library/js/pdbe-molstar-component-1.1.0.js"></script>
```

Until web components are natively supported by all browsers, it is necessary to use polyfills

Integration – PDBe Molstar

Step 2 : Create and render instance

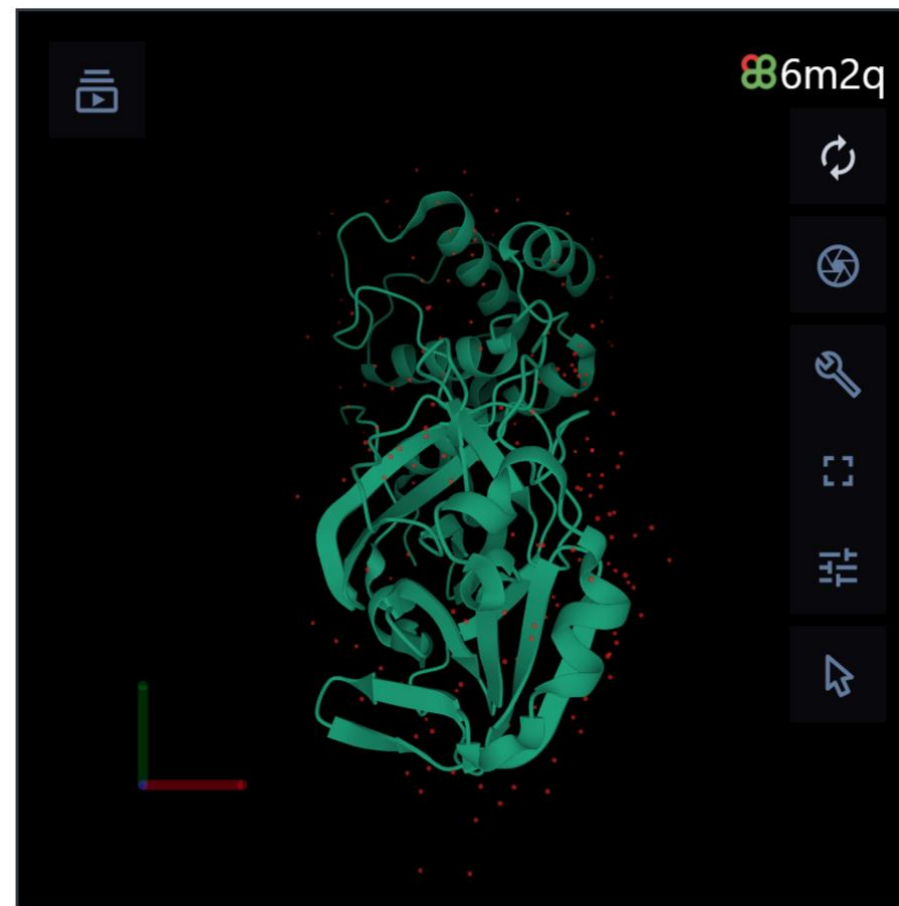
Plugin implementation: Instantiate plugin and provide parameters (options) to render

```
<script>
  //Create plugin instance
  const viewerInstance = new PDBeMolstarPlugin();

  //Set options (** All the available options are listed below in the documentation)
  const options = {
    moleculeId: '6m2q'
  }
  viewerInstance.render(viewerContainer, options);
</script>
```

Web component implementation: Include visualisation as HTML element

```
<pdbe-molstar molecule-id='6m2q'></pdbe-molstar>
```



pdbe.org/6m2q/3d

Integration – PDBe Molstar

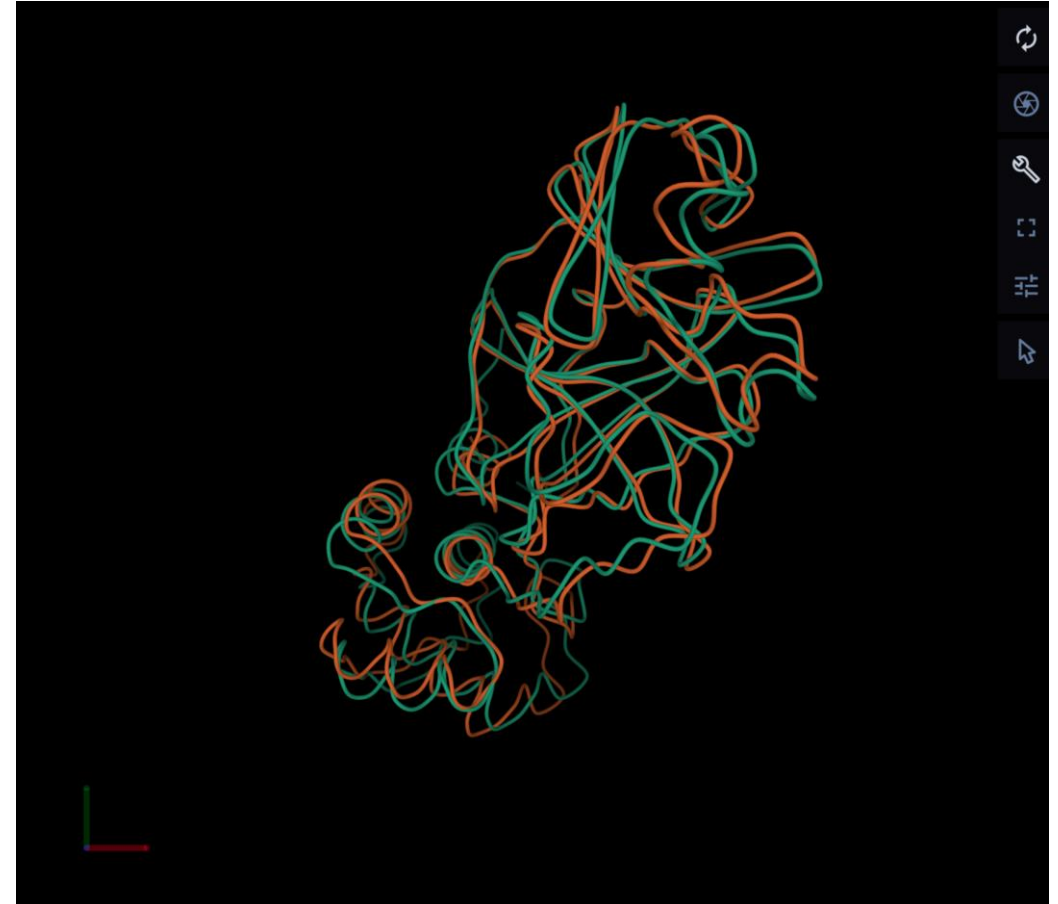
Customize using Parameters

```
<script>
  //Create plugin instance
  const viewerInstance = new PDBeMolstarPlugin();

  //Set options
  const options = {
    moleculeId: 'PRO_0000449623',
    superposition: true,
    superpositionParams: {
      matrixAccession: 'P0DTD1'
    }
  }

  //Get element from HTML/Template to place the viewer
  const viewerContainer = document.getElementById('myViewer');

  //Call render method to display the 3D view
  viewerInstance.render(viewerContainer, options);
</script>
```



Checkout <http://bit.ly/PDBe-superimposition-news> for more information on Superposition feature

Integration – PDB ProtVista

PDBe implementation of EBI Nightingale visualisation web components

- <https://github.com/ebi-webcomponents/nightingale>

Include PDB ProtVista library files in the web application

```
<!-- Polyfills -->
<!-- Required for IE11 -->
<script src="https://cdn.jsdelivr.net/npm/babel-polyfill/dist/polyfill.min.js"></script>
<!-- Web component polyfill (only loads what it needs) -->
<script src="https://cdn.jsdelivr.net/npm/@webcomponents/webcomponentsjs/webcomponents-lite.js" charset="utf-8"></script>
<!-- Required to polyfill modern browsers as code is ES5 for IE... -->
<script src="https://cdn.jsdelivr.net/npm/@webcomponents/webcomponentsjs/custom-elements-es5-adapter.js" charset="utf-8"></script>

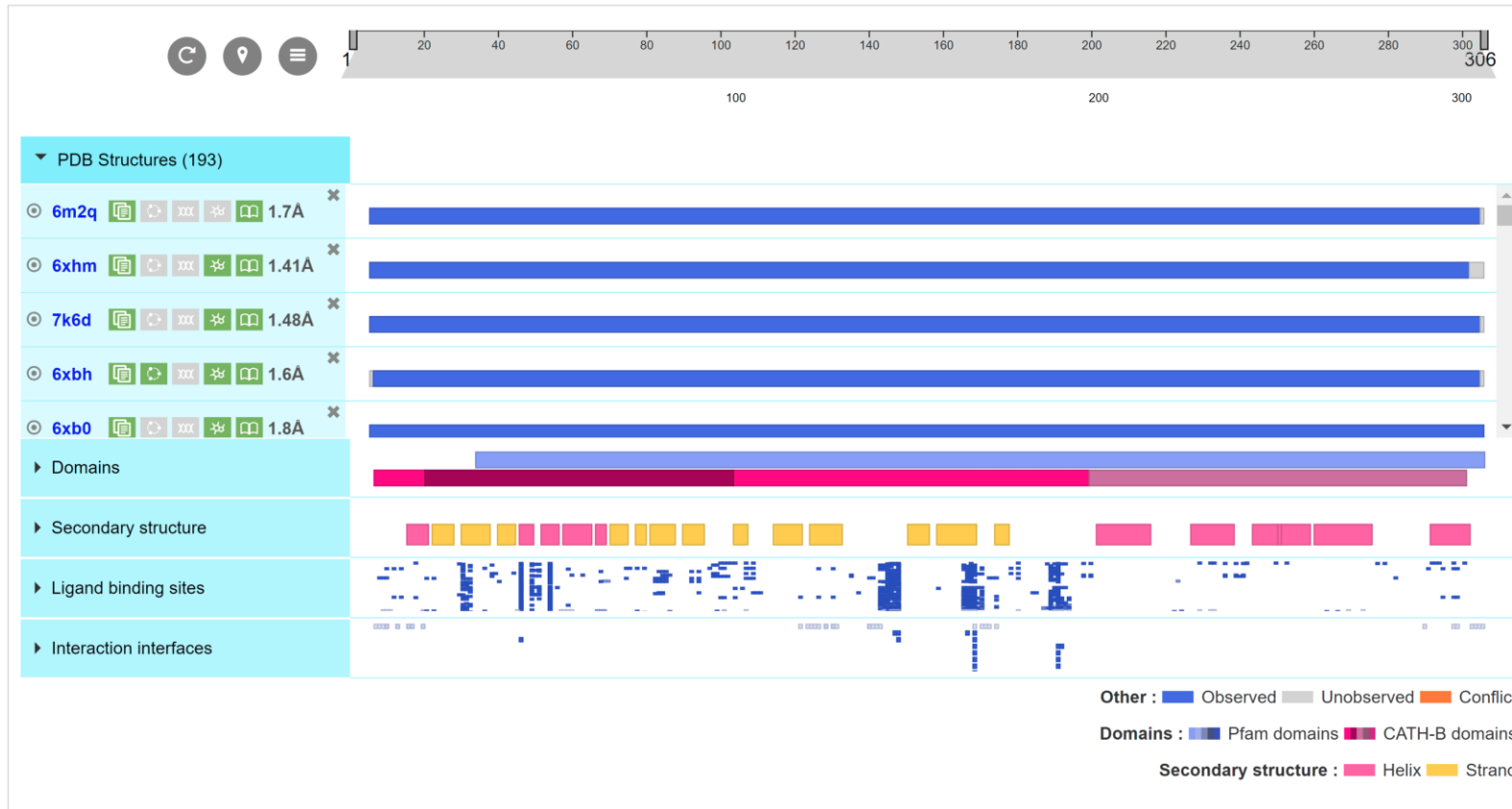
<!-- CSS -->
<link rel="stylesheet" href="https://ebi.emblstatic.net/web_guidelines/EBI-Icon-fonts/v1.2/fonts.css" type="text/css" media="all"/>

<!-- JS -->
<script src="https://d3js.org/d3.v4.min.js"></script>
<script src="https://www.ebi.ac.uk/pdbe/pdb-component-library/js/protvista-pdb-2.0.0.js"></script>
```

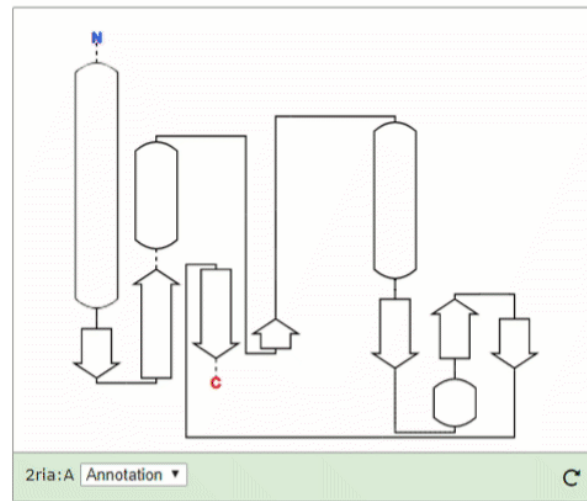
Integration – PDB ProtVista

Include PDB ProtVista web component in the application template

```
<protvista-pdb accession="PRO_0000449623"></protvista-pdb>
```



Interactivity



<https://www.ebi.ac.uk/pdbe/entry/pdb/2ria/protein/1>

Interactivity

Helper Methods allows programmatic control of the visualisation

```
<script>

// Focus (zoom-in) on chain A - residue 10-15
Instance.visual.focus([{"entity_id": "1", "struct_asym_id": "A", "start_residue_number": 10, "end_residue_number": 15}]);

// Highlight chain A residue 200-400 region
Instance.visual.highlight({ data: [{"entity_id": "1", "struct_asym_id": "A", "start_residue_number": 200, "end_residue_number": 400}] });

// Clear highlight
Instance.visual.clearHighlight()

</script>
```

All the methods are listed in the wiki documentation 'Helper Methods' section with details of expected parameter values and their data type

No.	Function	Parameters	Description
1	focus	<pre>params Type: json {"entity_id?": string, auth_asym_id?: string, struct_asym_id?: string, residue_number?: number, start_residue_number?: number, end_residue_number?: number, auth_residue_number?: number, auth_ins_code_id?: string, start_auth_residue_number?: number, start_auth_ins_code_id?: string, end_auth_residue_number?: number, end_auth_ins_code_id?: string, atoms?: string[], label_comp_id?: string}[]</pre>	<p>Focus on a particular visual section</p> <p>Example: <code>Instance.visual.focus([{"entity_id": "1", "struct_asym_id": "A", "start_residue_number": 10, "end_residue_number": 15}])</code></p> <p>will focus on residue range 10-15 of Chain 'A' of Entity 1</p>

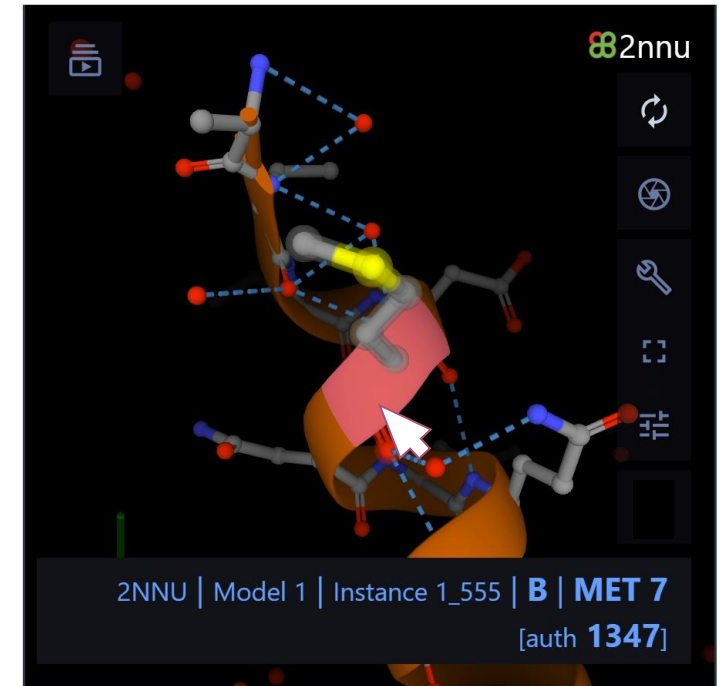
Interactivity

Custom Events to track mouse actions

```
<script>  
  document.addEventListener('PDB.molstar.click', (e) => {  
    //do something on event  
    console.log(e.eventData);  
  });  
</script>
```

Custom events are listed in the wiki documentation in 'Helper Methods' section

No.	Event	Description
1	PDB.molstar.click	Binds to click event. Event data (available in key = 'eventData') contains information structure residue clicked Example: <code>document.addEventListener('PDB.molstar.click', (e) => { //do something on event });</code>
2	PDB.molstar.mouseover	Binds to mouseover event. Example: <code>document.addEventListener('PDB.molstar.mouseover', (e) => { //do something on event });</code>
3	PDB.molstar.mouseout	Binds to mouseout event. Example: <code>document.addEventListener('PDB.molstar.mouseout', () => { //do something on event });</code>



```
▼ {  
  alt_id: ""  
  atom_id: "N"  
  auth_asym_id: "B"  
  auth_seq_id: 1347  
  comp_id: "MET"  
  entity_id: "2"  
  entry_id: "2NNU"  
  ins_code: ""  
  label_asym_id: "B"  
  seq_id: 7  
  ...}
```

Contact us!

 pdbhelp@ebi.ac.uk

 [GitHub/issues](#)



 Watch ▼

 Star

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Thank You!

Webinar series resources:

<https://pdbeurope.github.io/api-webinars>

<https://www.youtube.com/user/ProteinDataBank>

PDB Component Library:

<https://www.ebi.ac.uk/pdbe/pdb-component-library>

Component Library Collaborations:



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