



RBVI

# Displaying, Defining and Calculating Attributes

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## Notes



## Overview

- What are attributes?
- Depicting attributes graphically
- Selecting atoms, residues and molecules using attribute values
- Using Chimera tools to add new attributes
- Defining your own attributes

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## Notes



## What Are Attributes?

- Attributes are values associated with atoms, residues and molecules
- Chimera knows a lot about some of them
  - Atomic coordinates for graphical display
  - Atom specifiers
- Chimera knows little about others
  - Only name and value
  - For example, PDB files include temperature factor and occupancy for atoms
  - Tools for manipulating these attributes can:
    - depicting attributes graphically (e.g., by color)
    - select atoms with chosen range of attribute values

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# Using Attributes

- Graphical interface
  - Tools → Structure Analysis → Render by Attribute
- Command line interface
  - Atom specifier
    - color blue @/bfactor > 50
    - select @/ca/bfactor < 50
  - Command
    - rangecolor bfactor 0 blue 50 yellow 75 red
  - Both
    - rangecolor bfactor 0 blue 50 yellow 75 red @/ca

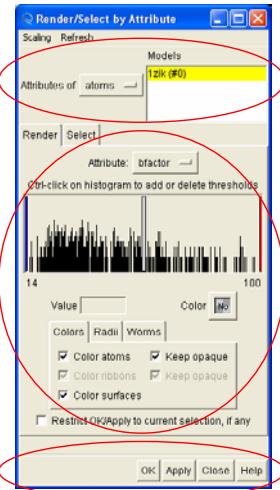
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# Render by Attribute

- Top section selects which attributes to use
- Middle section sets action type (changing graphical rendering or selection) and parameters
- Bottom buttons apply the action and/or closes the panel



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# Changing Graphical Rendering

- Change colors
  - Select attribute to map
  - Use histogram to select thresholds and associated colors
    - Control-click to add or remove thresholds
  - Choose which colors (atoms, ribbons and/or surfaces) to change
    - “Keep opaque” discards transparencies in colors specified in histogram
    - If some atoms have no values for the selected attribute, a, you can choose the default color for these atoms
  - Click “Apply” to update display

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# Changing Graphical Rendering

- **Changing atomic radii**
  - Select attribute to map
  - Use histogram to select thresholds and associated radius
    - Control-click to add or remove thresholds
  - Choose atom rendering style
    - If some atoms have no values for the selected attribute, a, you can choose whether radii of these atoms should change, and (if yes) the default radius
  - Click “Apply” to update display

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# Changing Graphical Rendering

- “Worms”
  - Displaying ribbons whose size is a function of attribute values
    - Only works with residue attributes
  - Use histogram to select thresholds and associated radius
    - Control-click to add or remove thresholds
  - Choose ribbon rendering style
    - Choose “non-worm” to go back to default ribbons
  - Click “Apply” to update display

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# Changing Selection

- Click the “Select” tab
- Use histogram to set a minimum and a maximum value
- Choose whether values between or outside the extrema should be selected
- Click “Apply” to update selection

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## Adding Attributes

- Some attributes (e.g., temperature factor) are read in as part of data files
- Chimera has tools that add attributes to open models:
  - MAV adds “mavPercentConserved” attribute
  - “Tools → Surface/Binding Analysis → Surface Area/Volume” adds surface area and volume attributes using the NCBI StrucTools server
- Once created, these attributes can be manipulated the same way as read-in attributes

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## Adding Your Attributes

- Attributes can be added using a text file with information on attribute name and what objects (atoms, residues or models) are affected
- Atom specifiers are used to assign values to matching objects

```
# Assign atomic weights to atoms
attribute: aw
match mode: any
recipient: atoms
    @/element="H"    1.00794
    @/element="C"    12.0107
    @/element="N"    14.0067
    @/element="O"    15.9994
    @/element="P"    30.973761
    @/element="S"    32.06
```

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## Adding Your Attributes

- Graphical interface
  - Tools → Structure Analysis → Define Attributes
- Command line interface
  - `defattr filename`
  - `defattr filename spec atom_specifier`

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# Calculating Attributes

- Attributes can be created by combining other attributes using **Tools** → **Structure Analysis** → **Attribute Calculator**
- Currently, only arithmetic operators, sum and average are supported

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## Summary

- Chimera has tools for manipulating “generic” attributes
  - Tools are in category **Structure Analysis**
  - **Render by Attribute** may be used to change graphical rendering and to select atoms, residues and models
  - **Define Attributes** and **Attribute Calculator** may be used to add new attributes

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