



Displaying, Defining and Calculating Attributes

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Notes

This image shows a single sheet of white paper with horizontal ruling lines. The lines are evenly spaced and run across the width of the page. There are no margins, text, or other markings on the paper.



- 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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- 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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Notes

[illegible]



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

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- 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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- 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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