

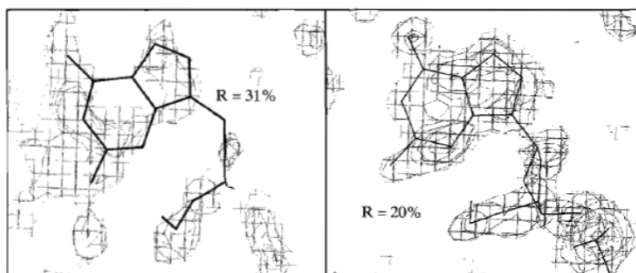
# The PDB and Molecular Visualization

Biochemistry Boot Camp  
Session #7  
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## Properties of PDB Files

- Experimental methodology:
  - X-Ray: Typically more precise
  - NMR: Need lots of “restraints;” sometimes hard to assess quality
- Most PDB files are solved using X-ray crystallography
  - 105,000 structures total
  - 89,000 are crystal structures

## Building an X-Ray Structure



**Figure 6.31** Effect of refinement on structure. The guanine nucleotide of a DNA fragment is shown with its electron density map prior to refinement and after refinement. Prior to refinement, the *R* factor is 31%. The structure is refined against the data to an *R* factor of 20%, which is one criterion of a good fit of the model to the data.

- **At first:** look for gross structural features (helix, backbone), then add side chains
- Molecular mechanics are used to help refine positions

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## Guidelines for X-Ray Quality

- **R-factor:** Less than 25% (ideally, less than 20%)
- **R-Free:** Bigger than R, but smaller than 25%
- **Resolution:** Less than 2.5 Å, but think about how much you need (1.5 Å usually very good)
  - At ~1 Å hydrogens become visible
- **Validation:** No clashes, good torsions, etc.
- **Water:** 2-5 molecules / kDa

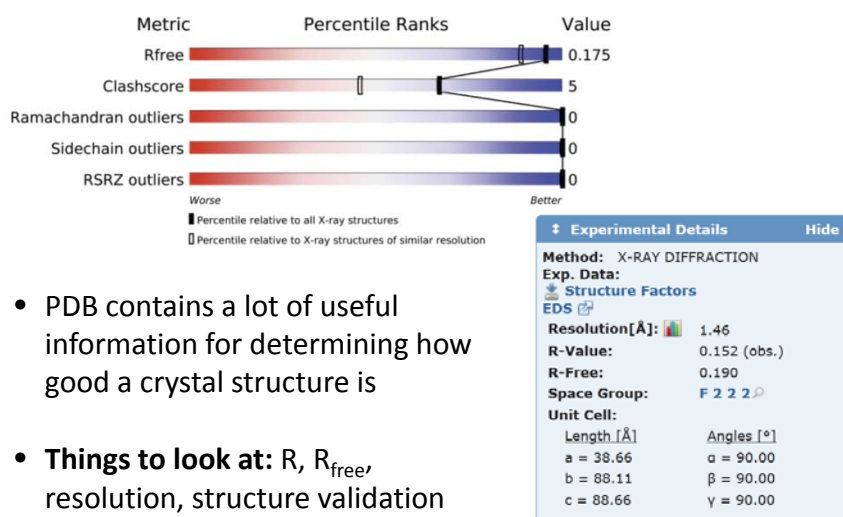
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## Protein Data Bank Revisited

- <http://rcsb.org/>
- **Input:** Protein name, PDB ID, authors, etc.
- **Output:** 3D coordinates of protein structures
  - Author information on methods
  - Cofactors and other information

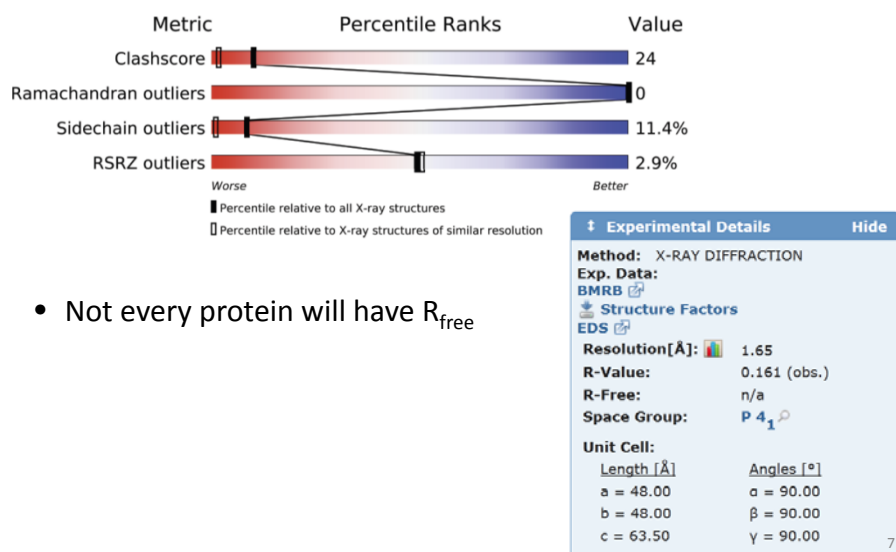
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## Assessing a Crystal Structure: 3TJW



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## Assessing a Crystal Structure: 1SNC



- Not every protein will have  $R_{\text{free}}$

## PDB Files: A Second Look

## Obtaining PyMOL

- Do NOT use the most recent educational release (1.7.4.4). It's buggy, and critical features (like ray tracing) are disabled.
- Older educational builds can be obtained by registering at:  
<http://www.pymol.org/educational/>
- I recommend version 1.3r1, although some features are still buggy (e.g. torsion angle calculation)

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## Obtaining PyMOL

- For Boot Camp, you can download PyMOL versions here (version 1.3r1):
- Windows: <http://goo.gl/0mRH2O>
- Mac: <http://goo.gl/U68Hoc>
- Linux: <http://goo.gl/HMZvPU>
- PyMOL is open source, and an alternative is downloading compiled versions on Linux (e.g. `apt-get install pymol` on debian-based systems)

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## Summary

- PDB files are complex models, derived from experimental data
  - Need to assess these models, too
- Atom names and properties are stored in the PDB, can be used to investigate structures
- PyMOL can make interesting pictures, but it is also a very powerful analytical tool

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