

# Applications of *SnB* to Proteins

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# Outline of Talk

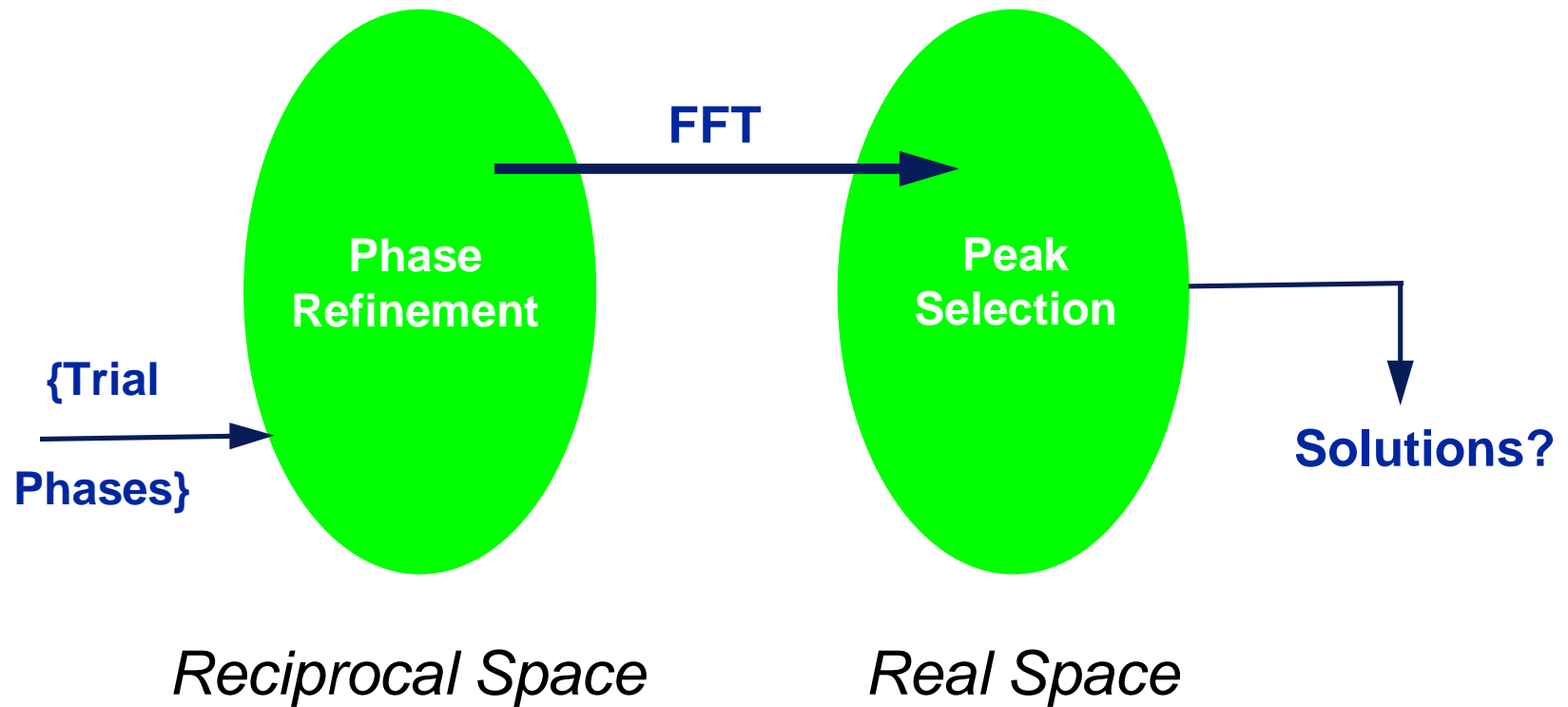
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*SnB*

- ◆ *Shake-and-Bake: The Method*
  - **Cyclical Procedure**
  - **The Minimal Function**
- ◆ *SnB: The Program*
- ◆ *Applications of SnB*
- ◆ *SnB version 2.0*

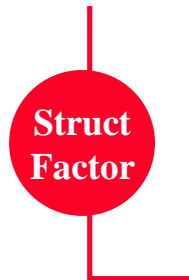
# Conventional Direct Methods

*SnB*



# *Shake-and-Bake*

{Trial  
Structures}



FFT<sup>-1</sup>



# *Shake-and-Bake*

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*SnB*

- ◆ **Direct Methods Optimization Technique**
- ◆ **Multiple Trial Structures**
- ◆ **Real Space  $\Leftrightarrow$  Reciprocal Space**
- ◆ **Phase Refinement Techniques**
  - **Parameter Shift (Minimal Function)**
  - **Tangent Formula**
- ◆ **Minimal Function as FOM**

# The Minimal Function

*SnB*

$$R = \frac{\sum_T W_T (\cos \phi_T - est_T)^2}{\sum_T W_T}$$

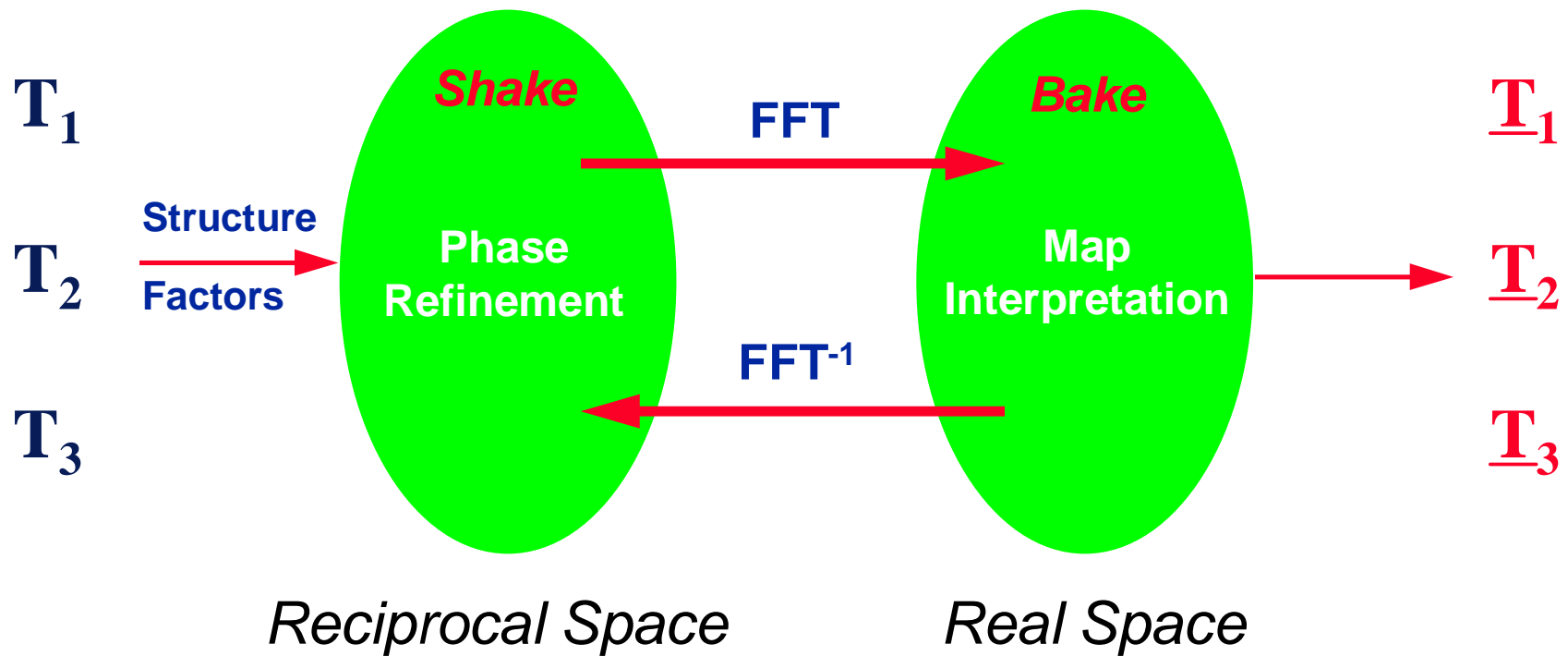
Triple:  $\phi_T = \phi_h + \phi_k + \phi_{-h-k}$

$$W_T = \left( \frac{2}{N^{1/2}} \right) |E_h E_k E_{-h-k}|$$

$est_T$  is the known expected value of  $\cos \phi_T$

# Shake-and-Bake

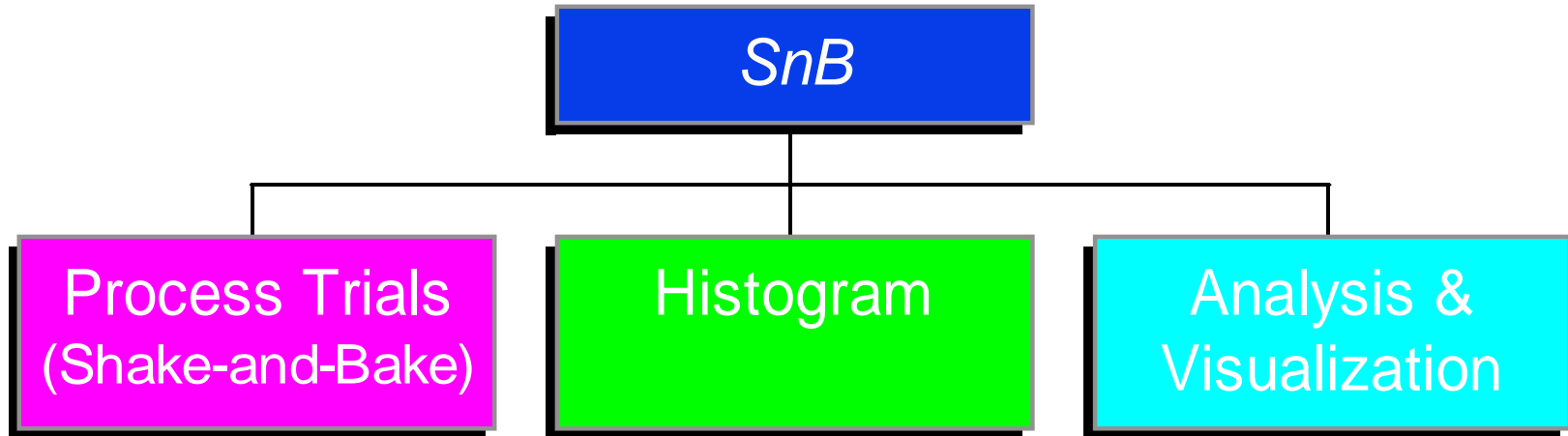
*SnB*



# Structure of *SnB*

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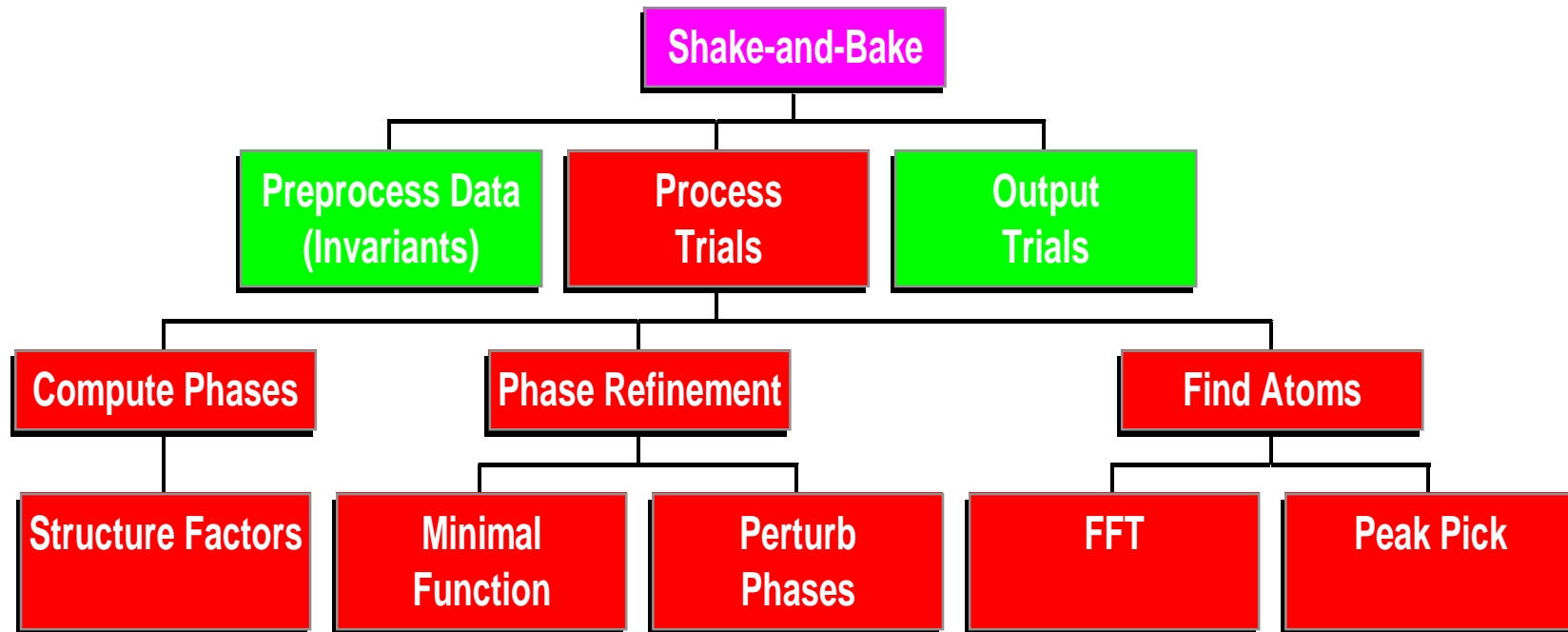
*SnB*





# Shake-and-Bake

*SnB*



# *SnB* Parameters

The logo for SnB, featuring the letters 'SnB' in a stylized, italicized font. The 'S' is red, the 'n' is grey, and the 'B' is red. The letters are slightly offset from each other, giving a 3D or layered appearance.

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	<b>Default</b>	<b>Ph8755</b>	<b>ToxII</b>
<b>Atoms (a.u.)</b>	<b>n</b>	<b>74</b>	<b>508</b>
<b>Phases</b>	<b>8n - 10n</b>	<b>740</b>	<b>5,000</b>
<b>Triples</b>	<b>70n - 100n</b>	<b>7,400</b>	<b>50,000</b>
<b>Cycles (PS)</b>	<b>n/2</b>	<b>40</b>	<b>255</b>
<b>Peaks recycled</b>	<b>0.8n - n</b>	<b>74</b>	<b>400</b>
<b>E-Fourier Steps</b>	<b>2</b>	<b>2</b>	<b>5</b>

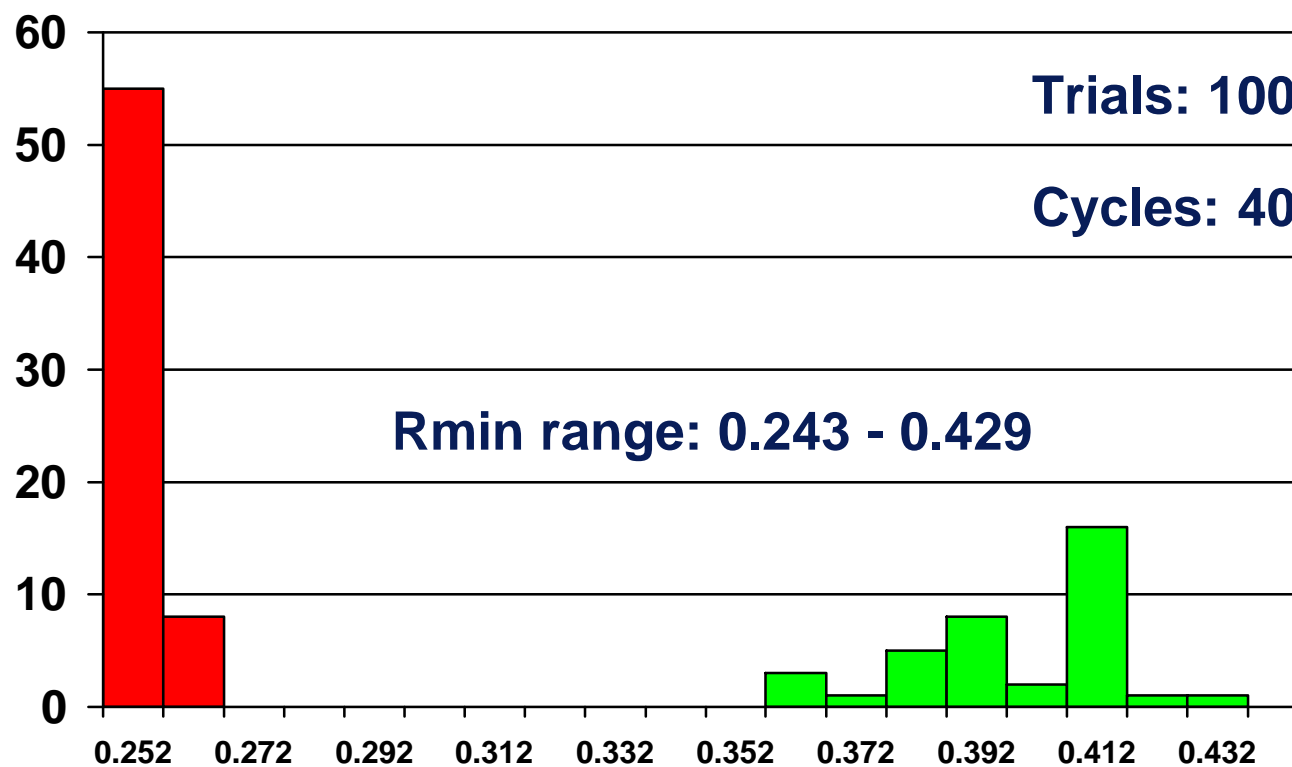
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# Sample Histogram (Ph8755)

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Atoms: 74  
Space Group: P1

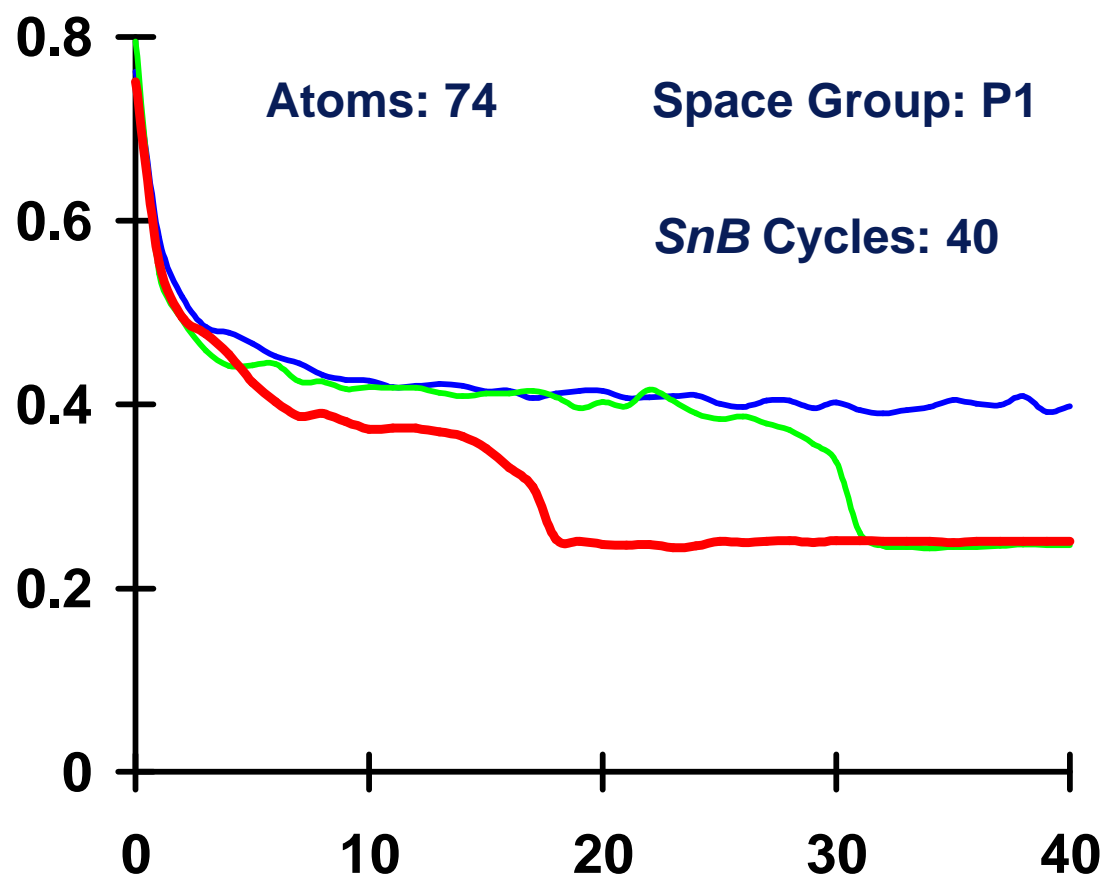
Phases: 740  
Triples: 7,400



# The Minimal Function is Diagnostic

Structure: Ph8755

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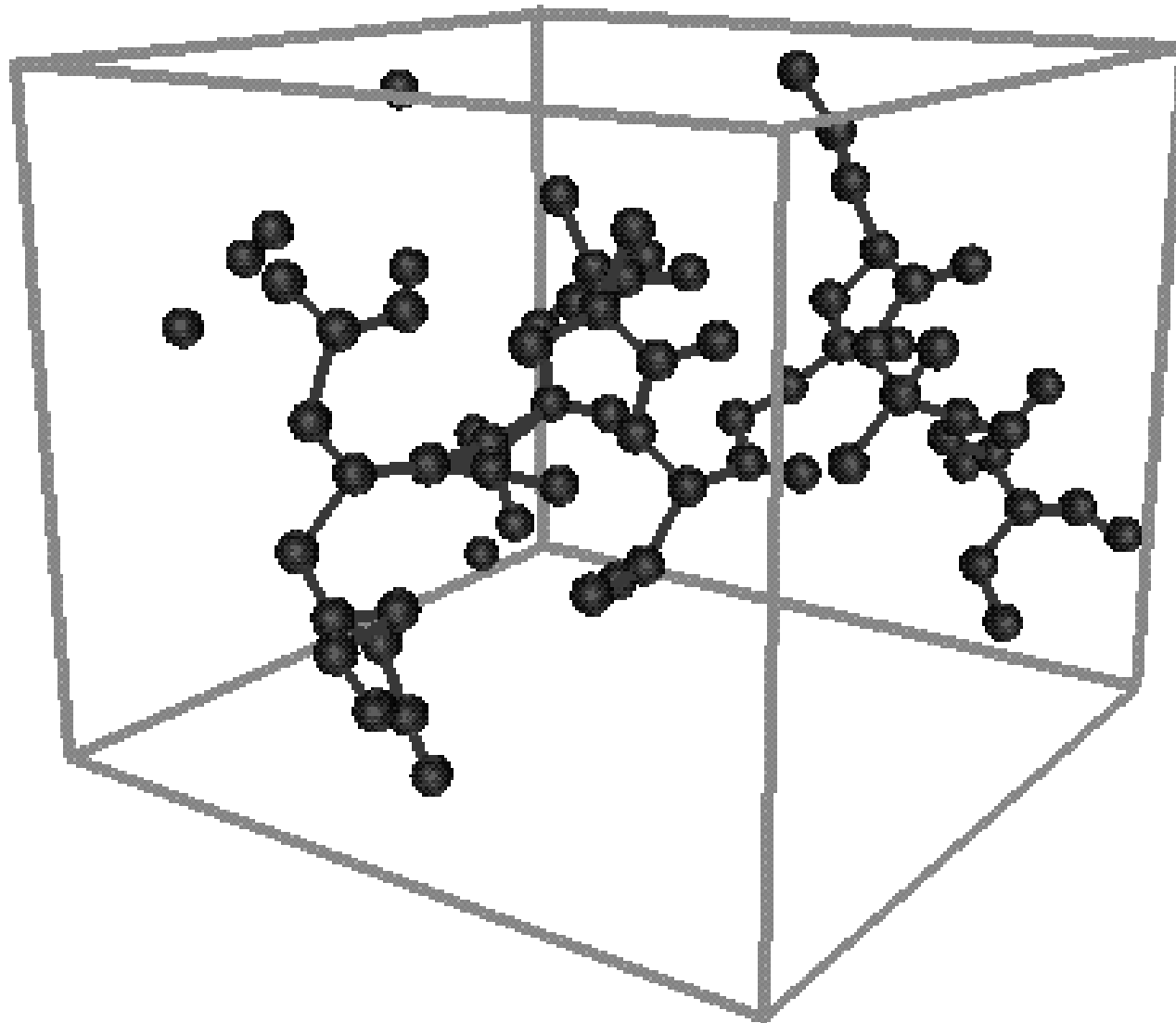


# Visualization in *SnB* (Ph8755)

*Geomview*: Geometry Center, U. Minn.

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# ToxII: *SnB* Histogram

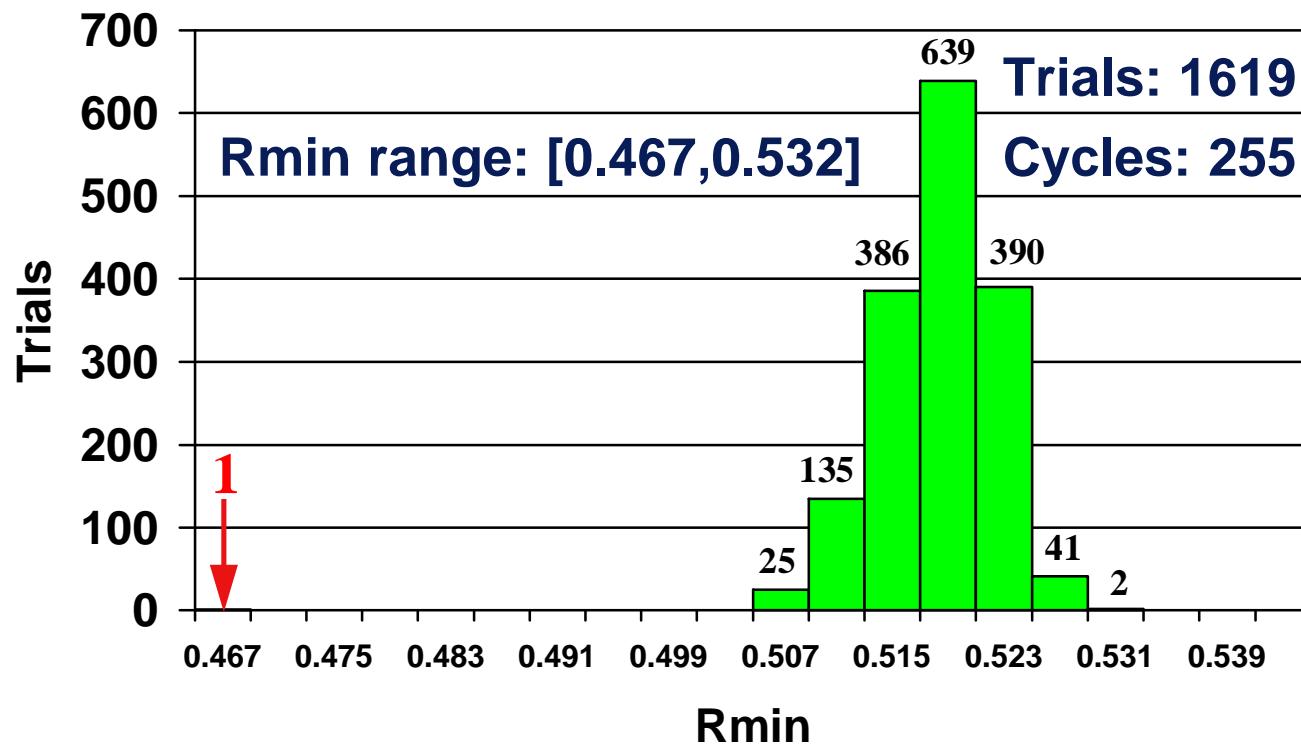
*SnB*

Atoms: 500

Phases: 5,000

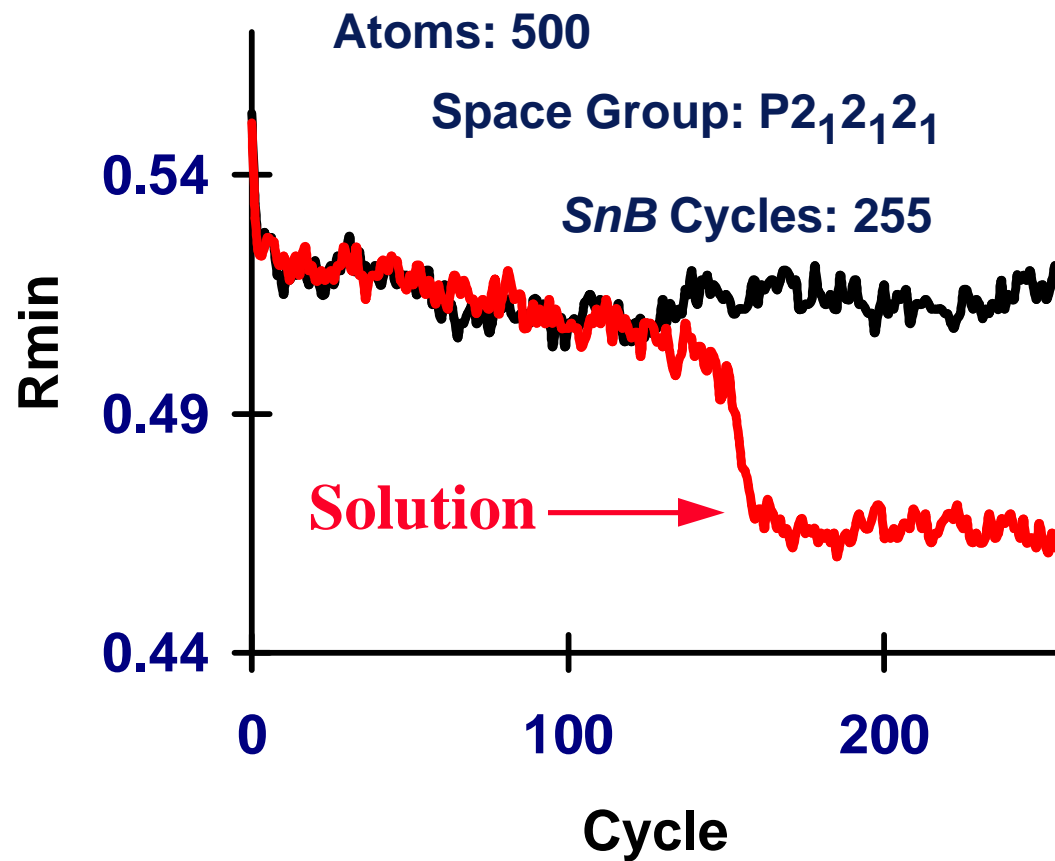
Space Group:  $P2_12_12_1$

Triples: 50,000



# Tox II: Trace of *SnB* Solution

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# Some *SnB* Solutions



STRUCTURE	LOCATION	ATOMS	SPACE GROUP
Scripps	Scripps	144	P1
Riboflavin tetrabutyrate	MSC	180	P1
Vancomycin	Penn	255	P <sub>4,2,2</sub>
Er-1 pheromone	UCLA	302	C2
Gramicidin A	HWI	317	P <sub>2,2,2</sub> <sub>1</sub>
Crambin	HWI	400	P <sub>2</sub> <sub>1</sub>
Alpha-1 peptide	OCI/U. of T.	450	P1
Rubredoxin	HWI	500	P <sub>2</sub> <sub>1</sub>
ToxII	HWI	630	P <sub>2,2,2</sub> <sub>1</sub>



# Computing Platforms

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*SnB*

## ◆ Unix Workstations

- ❑ SGI, Sun, DEC/Alpha
- ❑ IBM RS6000
- ❑ Wintel/Linux

## ◆ Parallel Computers

- ❑ Thinking Machines Corp. CM-5 (NCSA)
  - ❑ Cray T3D (PSC)
  - ❑ IBM SP2 (CTC)
- ## ◆ Cray C90 (PSC)

# Looking Ahead: *SnB* vers. 2.0

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- ◆ Includes Inverse FFT
- ◆ Additional Density Modification Options
- ◆ Improved Fourier Recycling: “Twice Baking”
- ◆ Input Improvements:  $|E|$  Calculation
- ◆ Output Improvements: Compatibility
- ◆ (SIR/SAS/MAD Invariants with est. values)

**PS02.03.16: Development of *SnB* Version 2**

# Related Presentations

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*SnB*

- ◆ **MS01.03.05:** Direct Methods Phasing of a 450 Atom Structure (Prive and Eisenberg)
- ◆ **MS02.06.07:** The *Ab Initio* Structure and Refinement of a Scorpion Protein Toxin (Smith, et. al.)
- ◆ **NO.BL.01:** The SAS Maximal Principle (Hauptman)
- ◆ **PS02.03.16:** Development of *SnB* Version 2 (Weeks and Miller)
- ◆ **PS02.06.09:** Application of the SAS Tangent Formula to Multiple Site Problems (Chang, et. al.)
- ◆ **MS02.01.05:** The Application of Shake and Bake to Unsolved Structures (Haltiwanger and Eggleston)

# Summary

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*SnB*

- ◆ *Shake-and-Bake*: Enhanced Direct Methods
- ◆ Targeted at 100-800 atom structures
- ◆ Publicly available
- ◆ Recommend: LEVY / EVAL (Bob Blessing)
- ◆ Current Research: *SnB* version 2.0
- ◆ Addresses:
  - <http://www.hwi.buffalo.edu/SnB/>
  - [snb-requests@hwi.buffalo.edu](mailto:snb-requests@hwi.buffalo.edu)
  - [snb-comments@hwi.buffalo.edu](mailto:snb-comments@hwi.buffalo.edu)

**SnB**

