Applications of *SnB* to Proteins

Russ Miller & Charles M. Weeks

Hauptman-Woodward Med. Res. Inst.

Principal Contributors:

C.-S. Chang	G.T. DeTitta	S.M. Gallo
H.A. Hauptman	H.G. Khalak	D.A. Langs
R. Miller	S. Potter	C.M. Weeks

Partial funding from NIH and NSF.

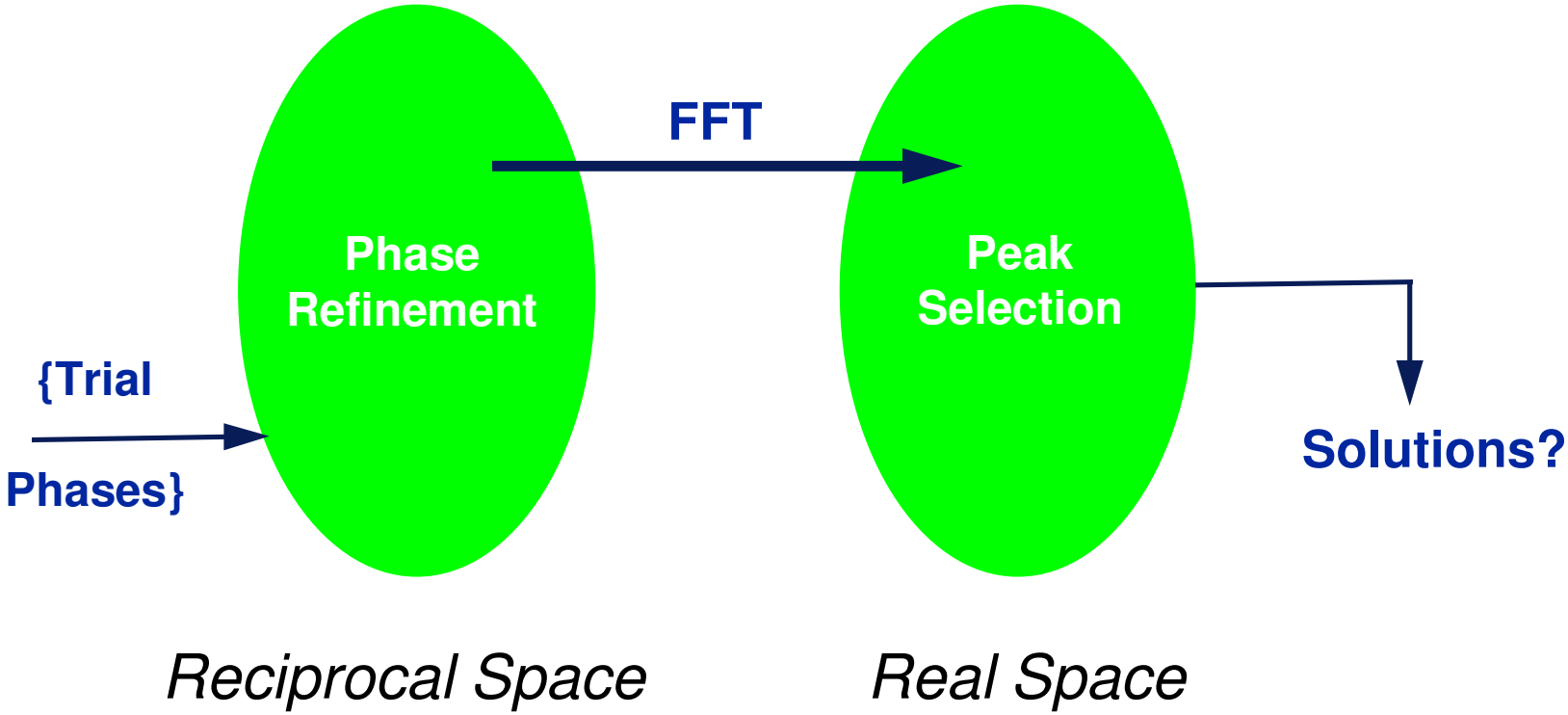
Outline of Talk

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

Shake-and-Bake

SnB

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

The Minimal Function

SnB

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

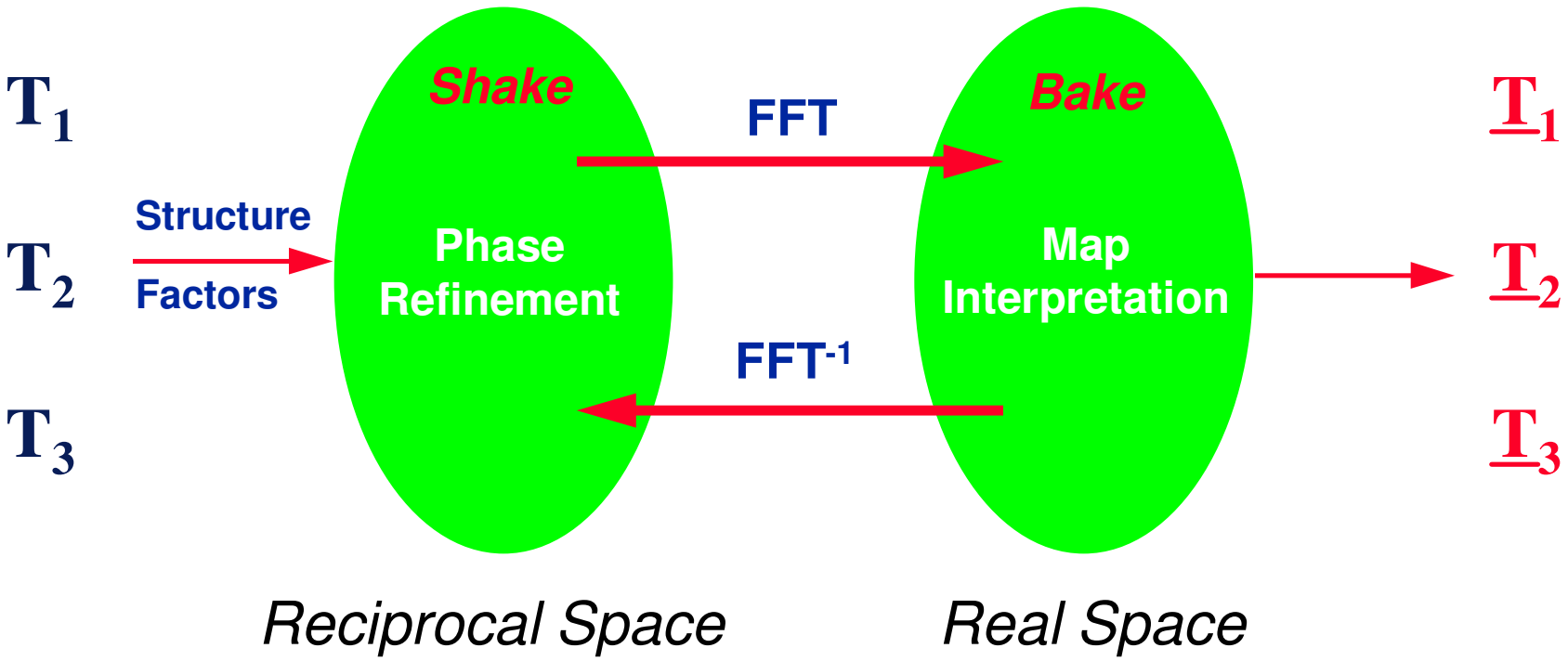
Triple: $\phi_T = \phi_h + \phi_k + \phi_{-h-k}$

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

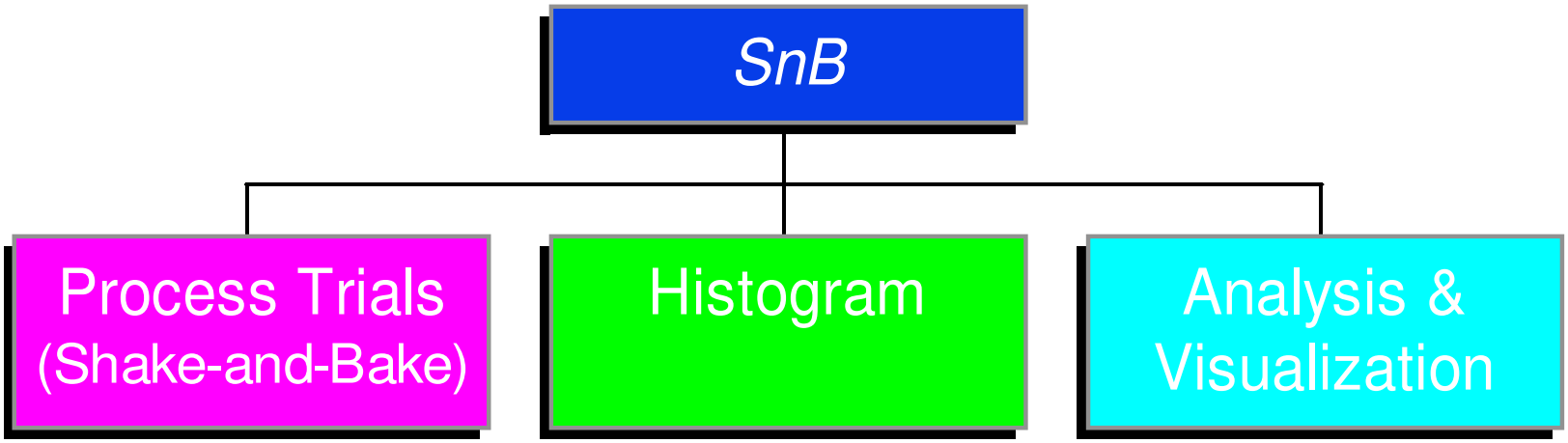
est_T is the known expected value of $\cos\phi_T$

Shake-and-Bake

SnB

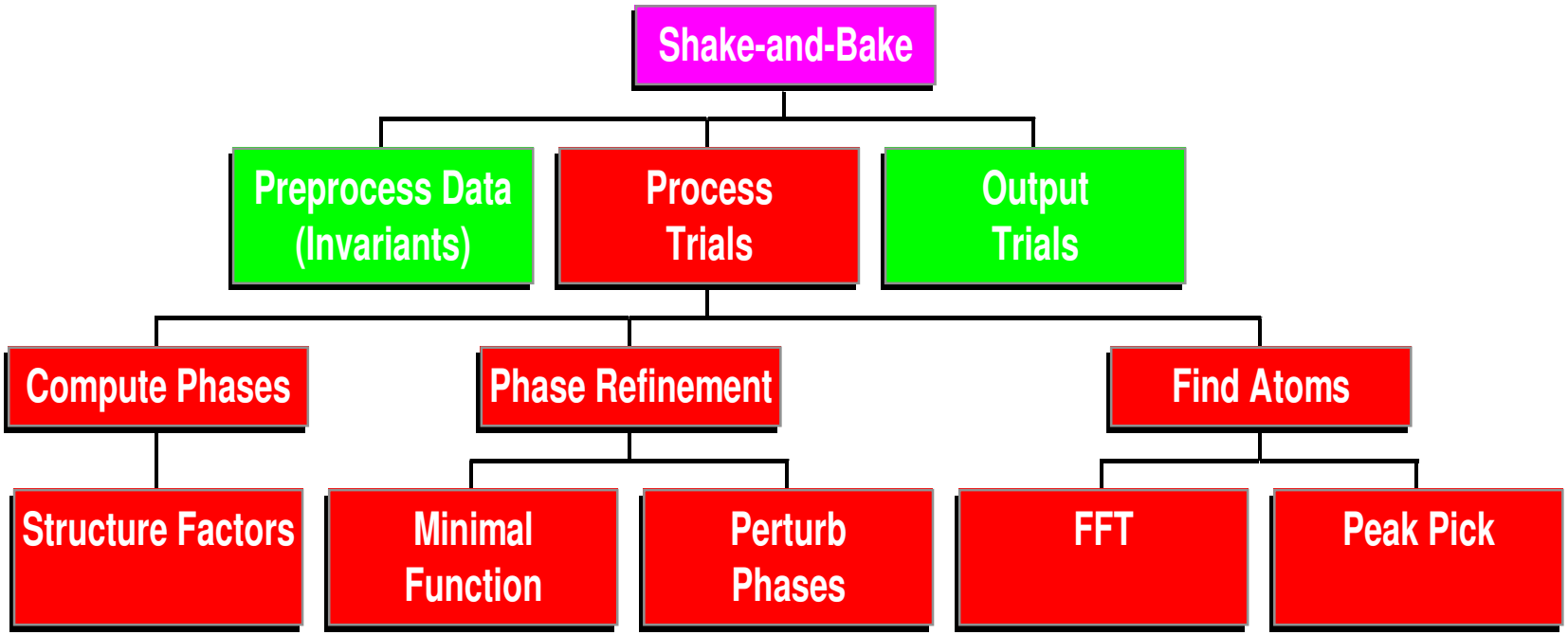


Structure of *SnB*



Shake-and-Bake

SnB



SnB Parameters

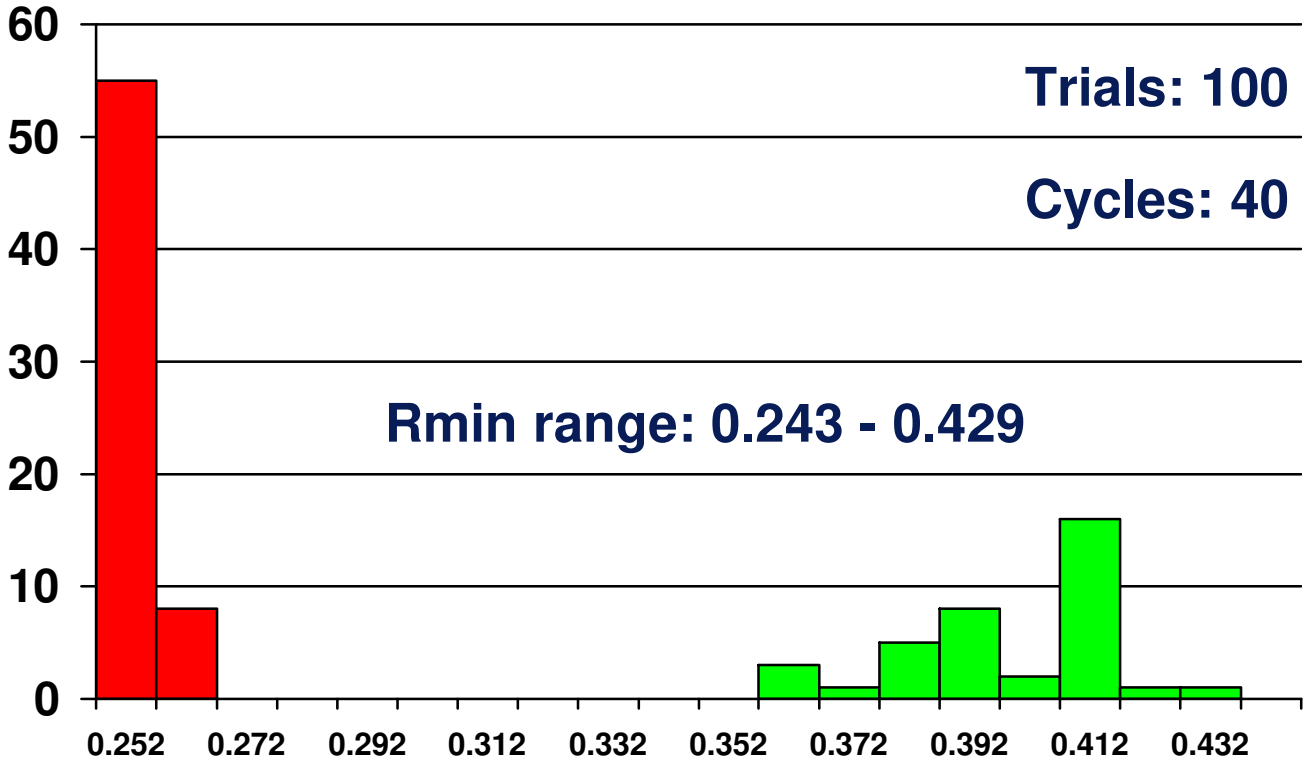
	Default	Ph8755	ToxII
Atoms (a.u.)	n	74	508
Phases	8n - 10n	740	5,000
Triples	70n - 100n	7,400	50,000
Cycles (PS)	n/2	40	255
Peaks recycled	0.8n - n	74	400
E-Fourier Steps	2	2	5

Sample Histogram (Ph8755)

SnB

Atoms: 74
Space Group: P1

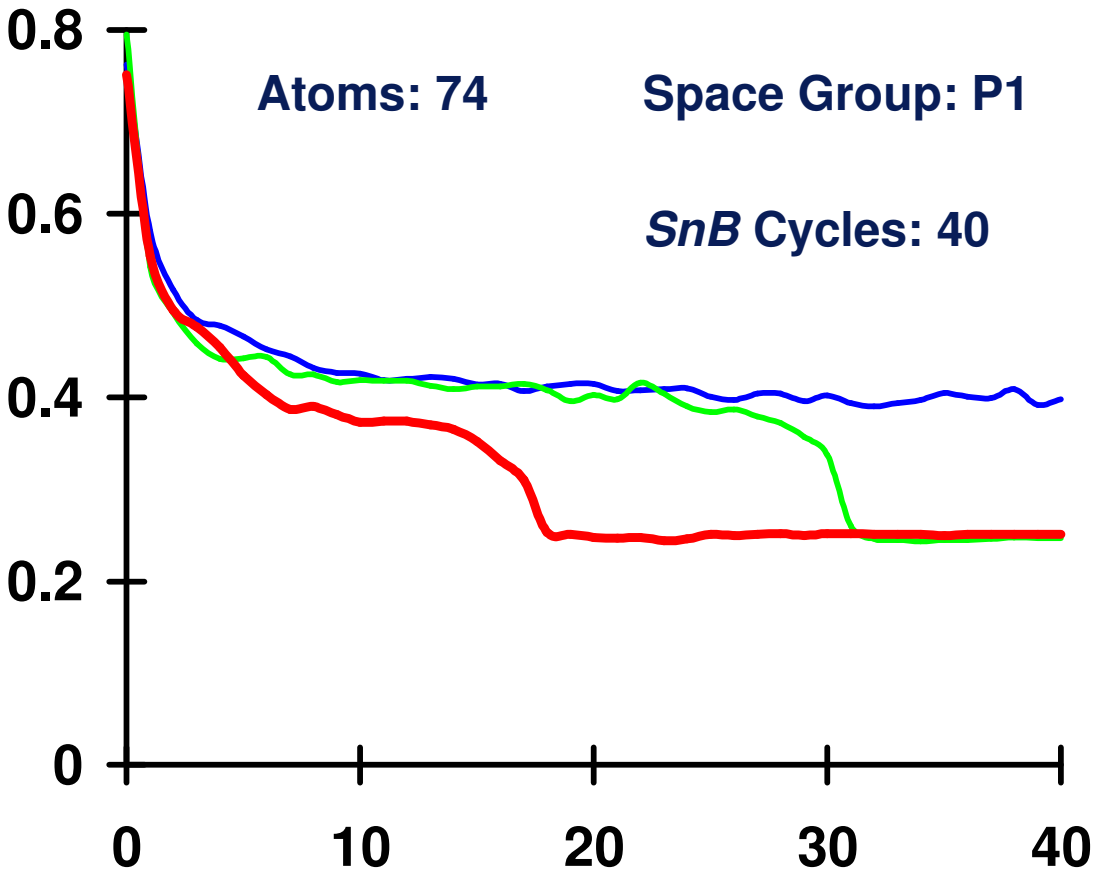
Phases: 740
Triples: 7,400



The Minimal Function is Diagnostic

Structure: Ph8755

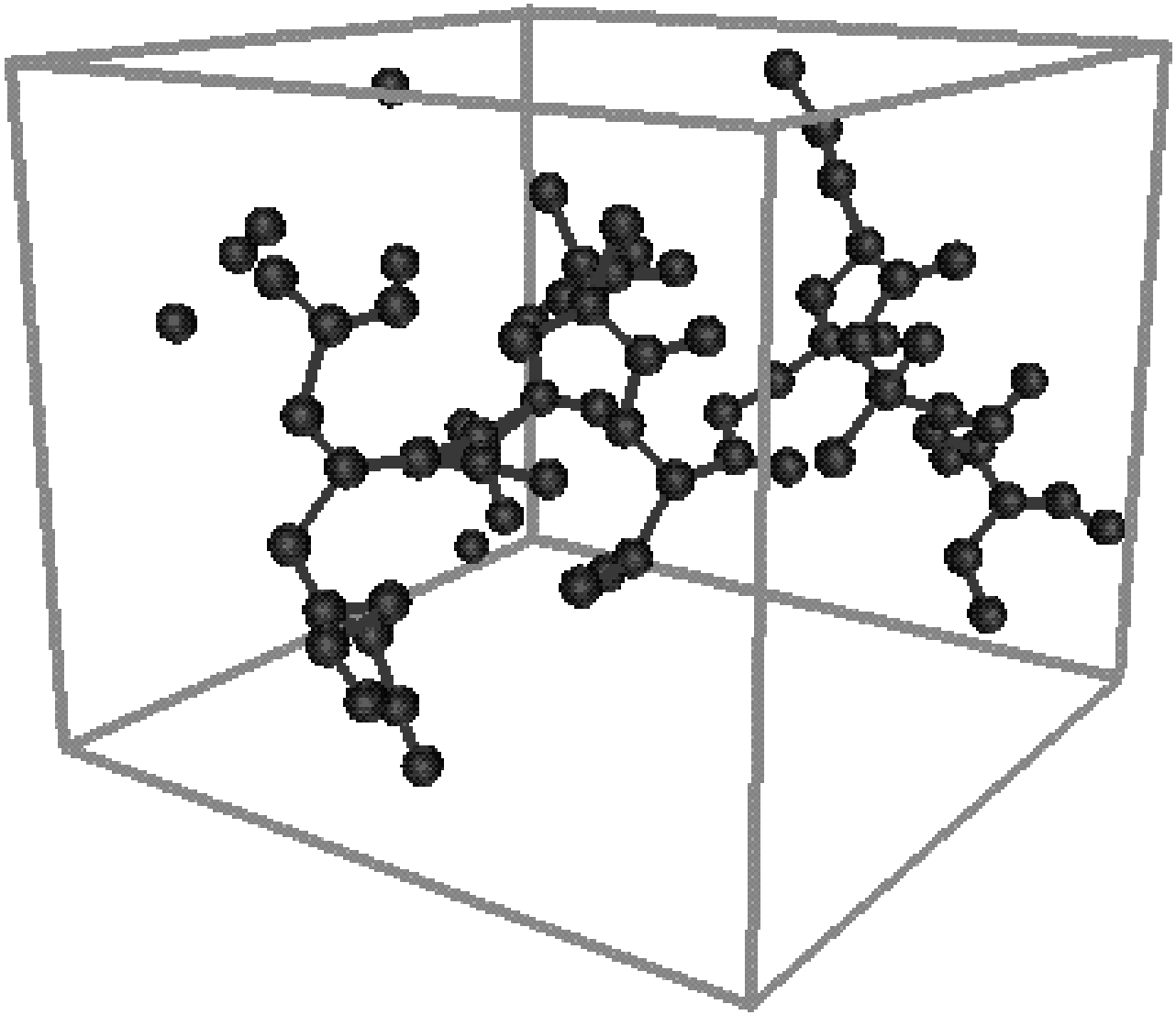
SnB



Visualization in *SnB* (Ph8755)

Geomview: Geometry Center, U. Minn.

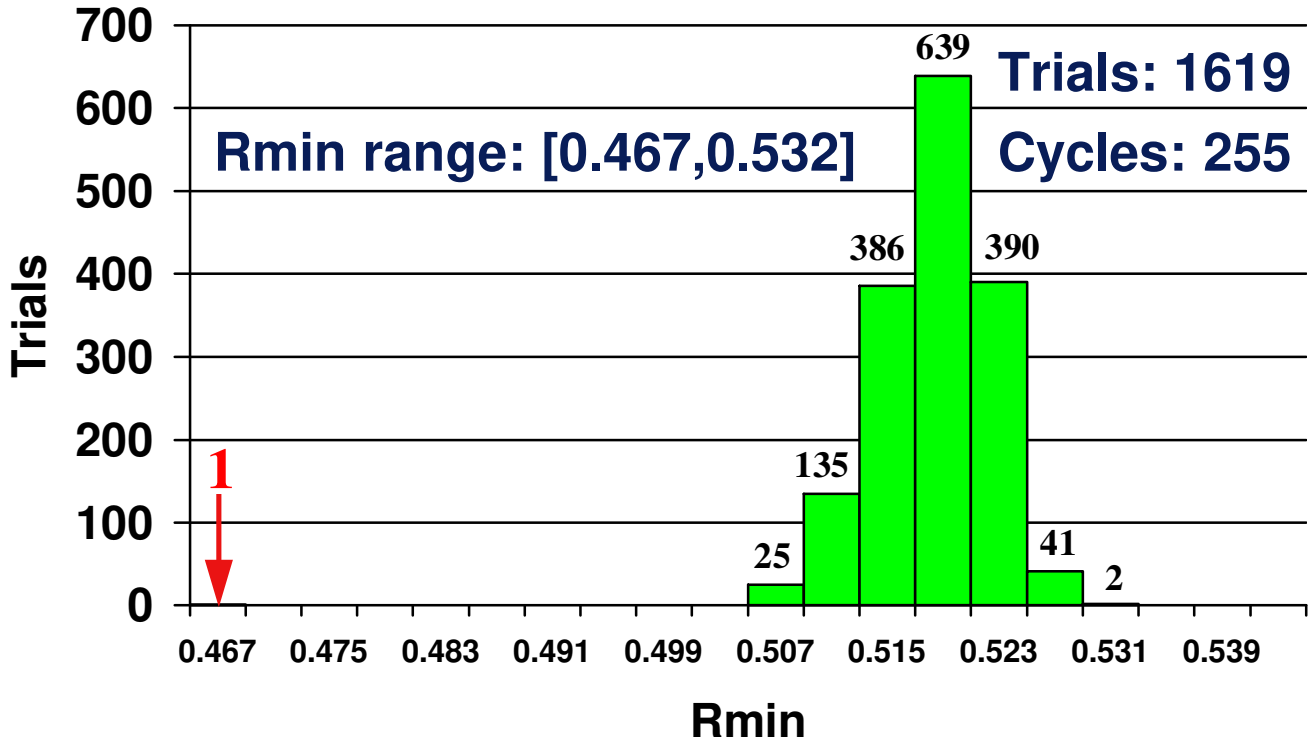
SnB



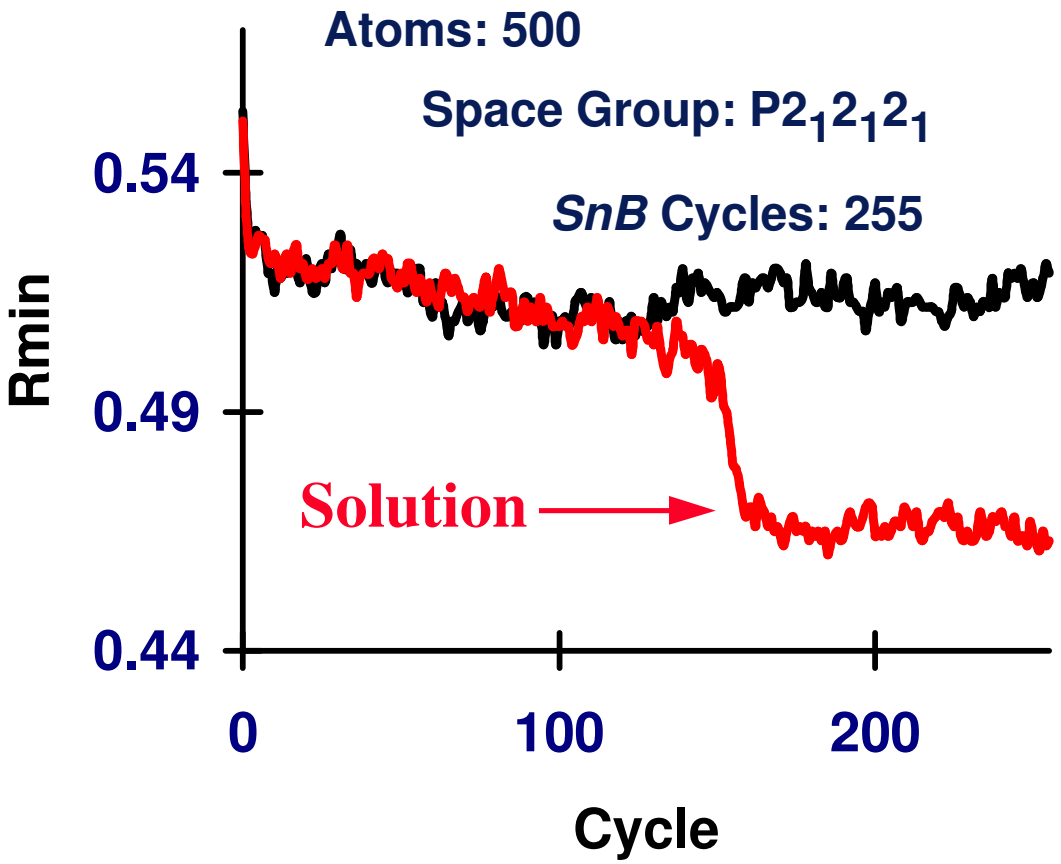
ToxII: *SnB* Histogram

Atoms: 500
Space Group: $P2_12_12_1$

Phases: 5,000
Triples: 50,000



Tox II: Trace of *SnB* Solution



Some *SnB* Solutions

Structure	Location	Atoms	Space Group
Scripps	Scripps	144	P1
Riboflavin tetrabutyrate	MSC	180	P1
Vancomycin	Penn	255	$P4_32_12$
Er-1 pheromone	UCLA	302	C2
Gramicidin A	HWI	317	$P2_12_12_1$
Crambin	HWI	400	$P2_1$
Alpha-1 peptide	OCI/U. of T.	450	P1
Rubredoxin	HWI	500	$P2_1$
ToxII	HWI	630	$P2_12_12_1$

Computing Platforms

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

- 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

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

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
  - snb-comments@hwi.buffalo.edu

SnB