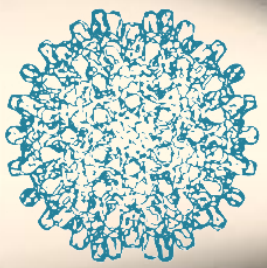
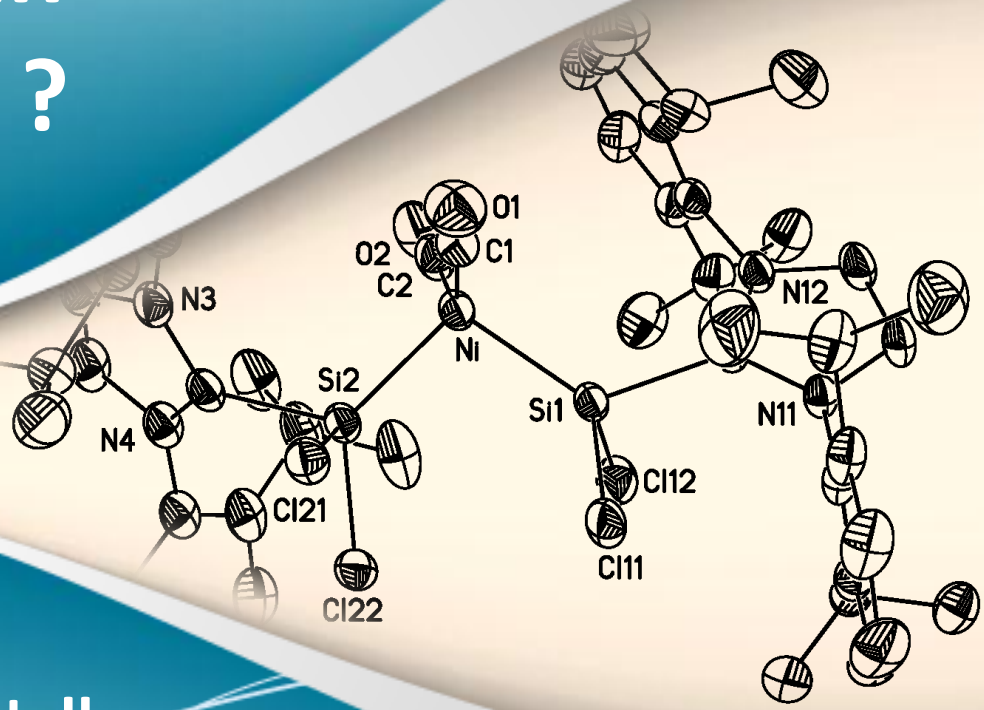
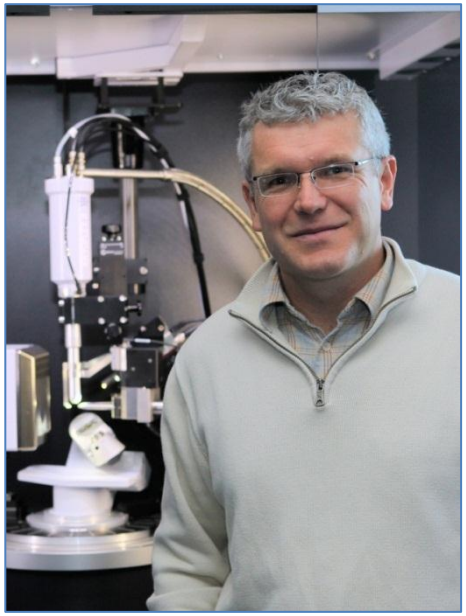
Bruker Webinar
What's new in SHELXL-2013 ?





Andrea Thorn
12th September, 2013
Michael Ruf & Bruce C. Noll

Welcome



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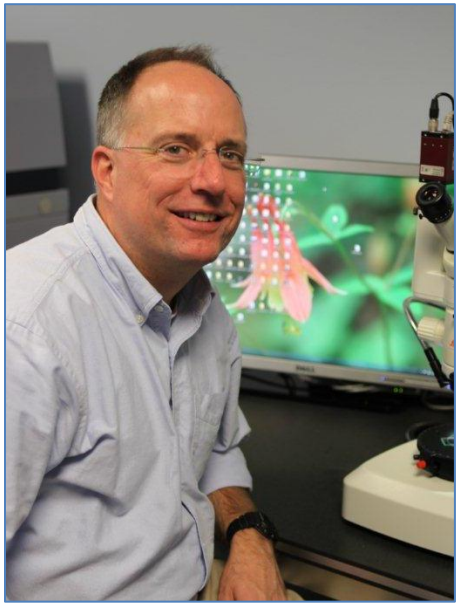

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Introduction: SHELXL_2013

- SHELXL_2013 is a program for the refinement of small and macromolecular crystal structures using single-crystal diffraction data from X-rays or neutrons.
- Stand-alone executables (no libraries, extra files or environment variables required).
- Compatible with all modern versions of Linux, Windows and MacOSX.
- Free for academic use.
- Compatible with SHELX76 and SHELXL-97.

Overview

Introduction

New features:

- Multiprocessor capability
- ADP restraints and constraints
- Neutron data refinement

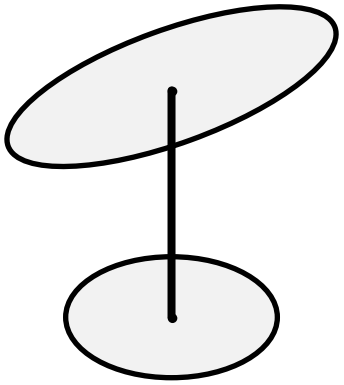
Remarks:

- Estimated standard deviations
- Absolute structure determination
- CIF matters
- Input and output

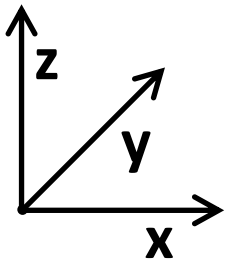
Rigid-bond restraints

Hirshfeld criterion for small molecule structure validation:

The mean-square displacement amplitudes of bonded atoms are equal in the direction of the bond joining them.



$\Delta U_{zz} = 0$



Hirshfeld, F. L. (1976). Acta Cryst. A32, 239–244.

Rigid-bond restraints

Rollett (1970): Rigid-bond restraints

`DELU`

- Improvement of the data/parameter ratio; enables **anisotropic refinement at relatively good resolution**.
- Standard deviation usually 0.01 - 0.001 $Å^2$
- Provides about one restraint per atom.
- If applied to 1,3-distances as well:

about two restraints per atom

Rollett (1970). ***Cryst. Computing,*** **167-181. Copenhagen: Munksgaard.**

Similar-U restraints

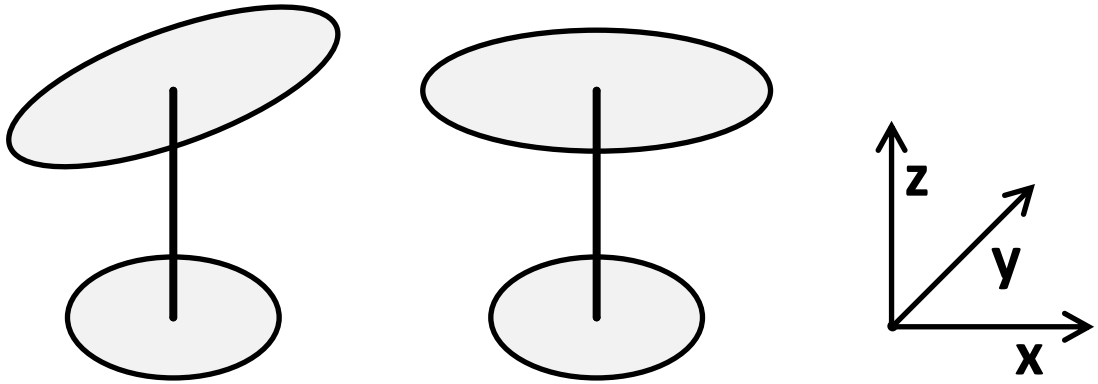
Similar U restraints: All six U_{ij} values of two bonded atoms should be as equal as possible.

`SIMU`

- Large estimated standard deviations
- Much less justified by theory and experimental evidence

Enhanced rigid-bond restraints

If a bond between two atoms is really rigid, the relative motion of the two atoms should be perpendicular to the bond!



$\Delta U_{zz} = 0$ $\Delta U_{zz} = 0$

$\Delta U_{yz} = 0; \Delta U_{xz} = 0$

Three restraints per atom; if applied to 1,3-distances: **Approximately 6 restraints per atom!**

Thorn, Dittrich, Sheldrick. (2012) Acta Cryst. A68, 448-451

Enhanced rigid-bond restraints

Enhanced rigid-bond restraint in SHELXL

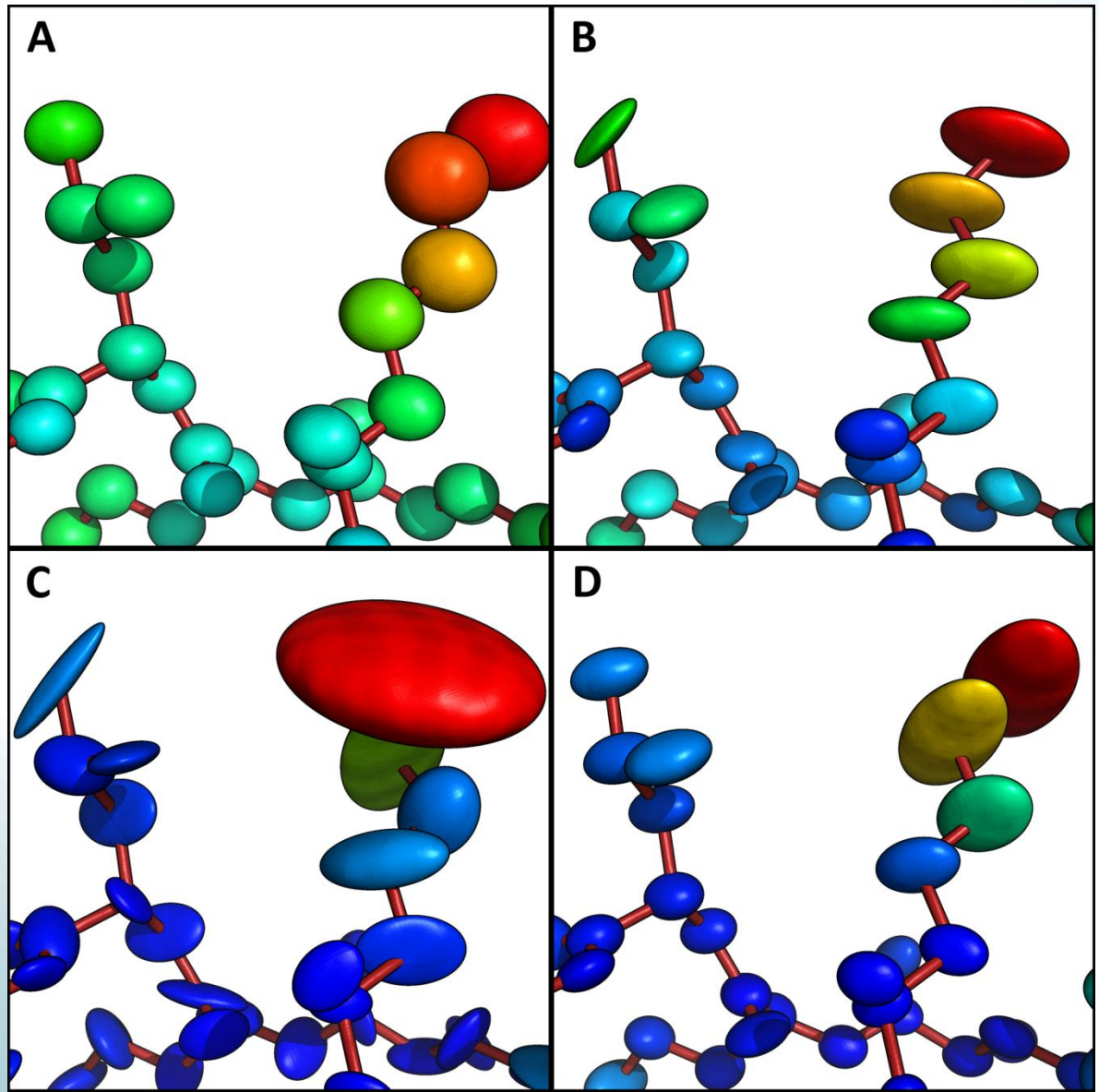
`RIGU`

Three restraints per atom; if applied to 1,3-distances:
Approximately 6 restraints per atom!

The **new rigid-bond restraints** are an enhancement to the established rigid-bond restraints. However, they cannot account for occupancies dropping along side chains, but may expose such defects.

Thorn, Dittrich, Sheldrick. (2012) Acta Cryst. A68, 448-451

Tests



PDB 1us0
at 1.7 Å

XNPD constraint

`XNPD [-0.001]`

- New constraint
- Lower bound for the eigenvalues of the U_{ij} tensor of all anisotropic atoms –
- or the U of isotropic atoms
- The slightly negative default ensures that NPD reports but the refinement does not blow up.

Hydrogen atoms and neutron diffraction

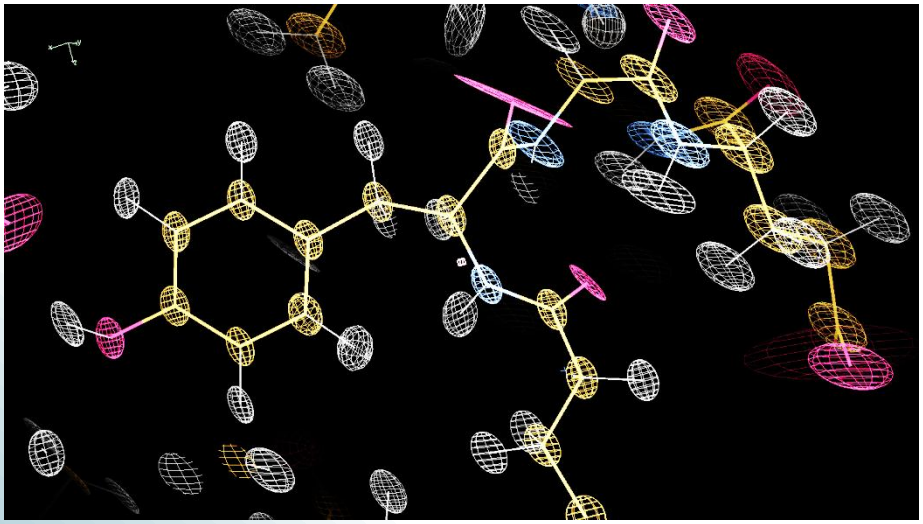
NEUT

To be inserted before **SFAC:** neutron scattering factors default **HFIX/AFIX** bond lengths are changed

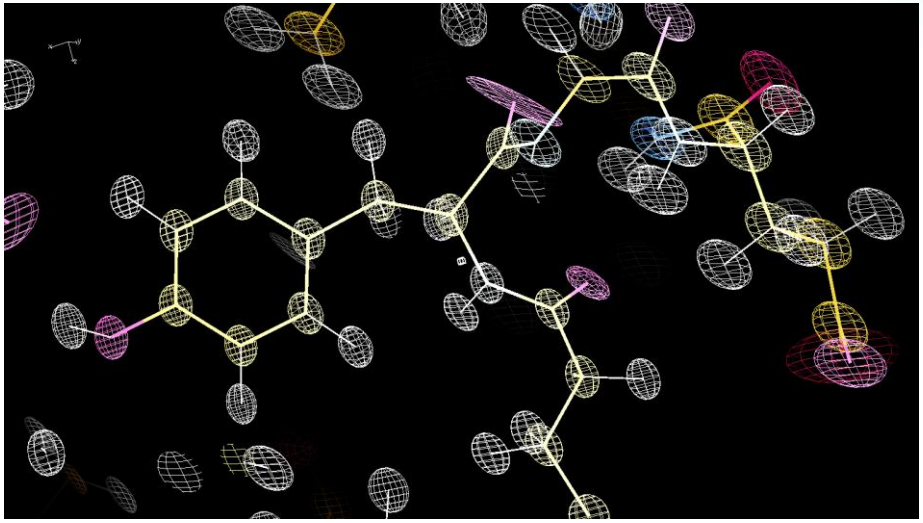
- H/D mostly treated as normal atoms, except for chiral volume restraints (**CHIV**) and riding model (**AFIX**).
- **DFIX and SADI distance restraints work better than the H or D riding model for neutron data.**
- If **CHIV** is applied to an atom that is bonded to exactly three non-H/D atoms, bonds to H/D are ignored.
  - Thus the same **CHIV** restraints can be used as for X-rays.
- For atoms bonded to 3 atoms including H/D, all are used.

Anisotropic hydrogens?!

RIGU works well for H/D when refining against neutron data, despite the poor data to parameter ratio, as shown below for myoglobin 1.5Å neutron data (PDB 1L2K).



RIGU + XNDP 0.001



RIGU + XNDP 0.001 + ISOR 0.04 0.04

With RIGU alone, atoms move at right angles to the bonds but ORTEPs are unreasonable. Correction with **ISOR**.

Anna Lübben and Tim Grüne

Estimated standard uncertainties

Standard uncertainties obtained by least-squares are proportional to

$$(N–P)^{-½}$$

N number of observations

P number of parameters

SHELXL _2013 implements a proposal by Ton Spek, that N should always be set to the number of unique reflections.

Estimated standard uncertainties

Consequences:

1. The e.s.d.s no longer depend on how data were merged. Unmerged data should be read into SHELXL for more complete statistics. **`MERG 4`** may still be used for macromolecules.
2. For HKLF5 twin refinements, ALL data can be used.
3. Some standard uncertainties may be slightly greater than before. They were probably underestimated.
4. The third L.S. parameter is no longer required (except for squeezed structures).

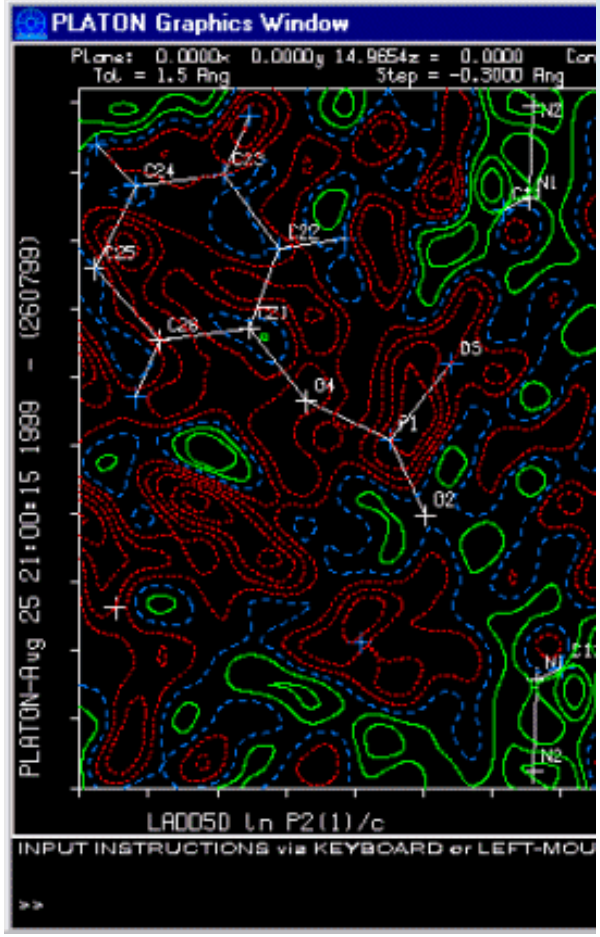
Additional structure factor contribution

ABIN

Input of A and B parts of a calculated structure factor:

- e.g. a *squeezed* region of the cell
- or a solvent mask contribution of a macromolecule

This is especially designed to be compatible with twinned refinements and with Ton Spek's PLATON.



Absolute structure determination

Absolute structure from weak anomalous signal:
SHELXL now calculates the Flack parameter by the Parsons' quotient method at the end of the refinement and outputs the results to the console, *.lst* and *.cif*, for example:

```
Flack x = 0.012 (14) from 271 selected quotients (Parsons' method)
```

Parsons, Flack & Wagner: Post-refinement against Friedel differences or quotients $Q = (I_+ - I_-) / (I_+ + I_-)$ gives much lower e.s.d.s than including the Flack parameter in the full-matrix refinement. The quotients cancel systematic errors (such as bonding electron density) that affect I_+ and I_- equally, and in SHELXL-2013 even give good results for twins.

Thompson & Watkin, *Tetrahedron Asymmetry*, 20 (2009) 712
Parsons, Flack & Wagner, *Acta Cryst.* B69 (2013) 249

CIF matters

SHELX-2013 contains extensive changes to its **CIF output** and should be fully compatible with core-CIF version 2.4.3.

The SHELXL-97 definition of *atom site multiplicity* was different to the IUCr definition. This has been fixed by calling the SHELX number *order* instead. Problems may still arise for disordered atoms or groups close to but not exactly on special positions, which is why SHELX never uses this concept (except for writing it to the CIF file).

Improving CIF as an archive format

The *.hkl* file (HKLF 3, 4 or 5 format) and *.res* file are now embedded into the *.cif* output file (with checksums). This makes it possible to repeat any refinement exactly, and discourages cosmetic editing.

- The program **ShredCIF** is provided for extracting the embedded files and verifying their checksums.

SHELXL now deduces the space group name and Hall symbol from LATT and SYMM, but only for 249 common settings. The space group is also written to a COOT-compatible *.pdb* file.

Further new features

- **HFIX** sometimes generates a few bad connectivity error messages when first applied. These are now all printed before aborting. They may then be fixed by **HFIX 0** (before the current **HFIX**s) or **FREE** or **BIND** instructions.
- **HTAB** without atom names now writes the appropriate **EQIV** and full **HTAB** instructions to the end of the *.res* file so that they can be used in the next refinement job. Non-classical C-H..O hydrogen bonds are also generated.
- **SADI** without atom names expands all **SAME** instructions into **SADI** and adds them at the end of the *.res* file.

ACKNOWLEDGEMENTS

George Sheldrick

The Crystallographic Computing group at the LMB –
Garib Murshudov, Rob Nicholls, Paul Emsley, Fei Long

Richard Cooper

The programs are **free for academic use:**
http://shelx.uni-ac.gwdg.de/SHELX/

SEVENTH FRAMEWORK PROGRAMME

MARIE CURIE ACTIONS

MRC | Laboratory of Molecular Biology

Standard deviations

Usage as restraint:

$$\frac{\sqrt{p^2+Ueq_{,A}+Ueq_{,B}}\,\sigma}{p} \qquad \frac{\sqrt{p^2+Ueq_{,A}+Ueq_{,B}}\,\sigma\, d}{p}$$

A and B are the two atoms

$\boldsymbol{U_{eq}}$ equivalent isotropic displacement parameter

$\boldsymbol{d}$ is the distance between atoms A and B

$\boldsymbol{\sigma}$ and $\boldsymbol{p}$ are user-supplied parameters

(0.004 Å^2 and p = 0.5 gave good results)

ADPs are not allowed to be non-positive definite.

Verification at high resolution

- Refinement of a cyclic hexapeptide
- 0.382 Å; 100 K
- Cut to 0.84 Å

	$IAM_{0.84}$ 1,2	IAM 1,2	XD 1,2	$IAM_{0.84}$ 1,3	IAM 1,3	XD 1,3
r.m.s. ΔU_{ZZ} [Å^2]	0.00165	0.00034	0.00031	0.00188	0.00074	0.00076
r.m.s. $\Delta U_{XZ\&YZ}$ [Å^2]	0.00258	0.00180	0.00183	0.00301	0.00242	0.00240
r.m.s. ΔU_{XY} [Å^2]	0.00406	0.00304	0.00304	0.00389	0.00386	0.00393
r.m.s. $\Delta U_{XX\&YY}$ [Å^2]	0.00665	0.00605	0.00600	0.00788	0.00761	0.00767

IAM = Independent atom refinement
XD = XD multipole refinement

Test set

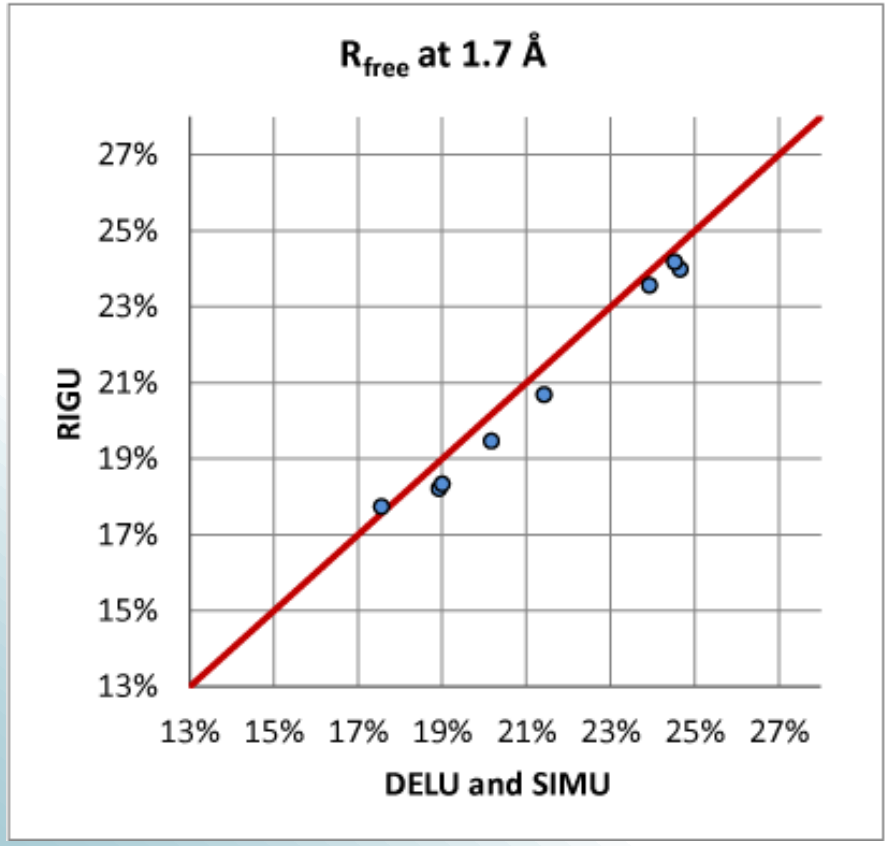
Test set: **Eight well-refined protein structures** *

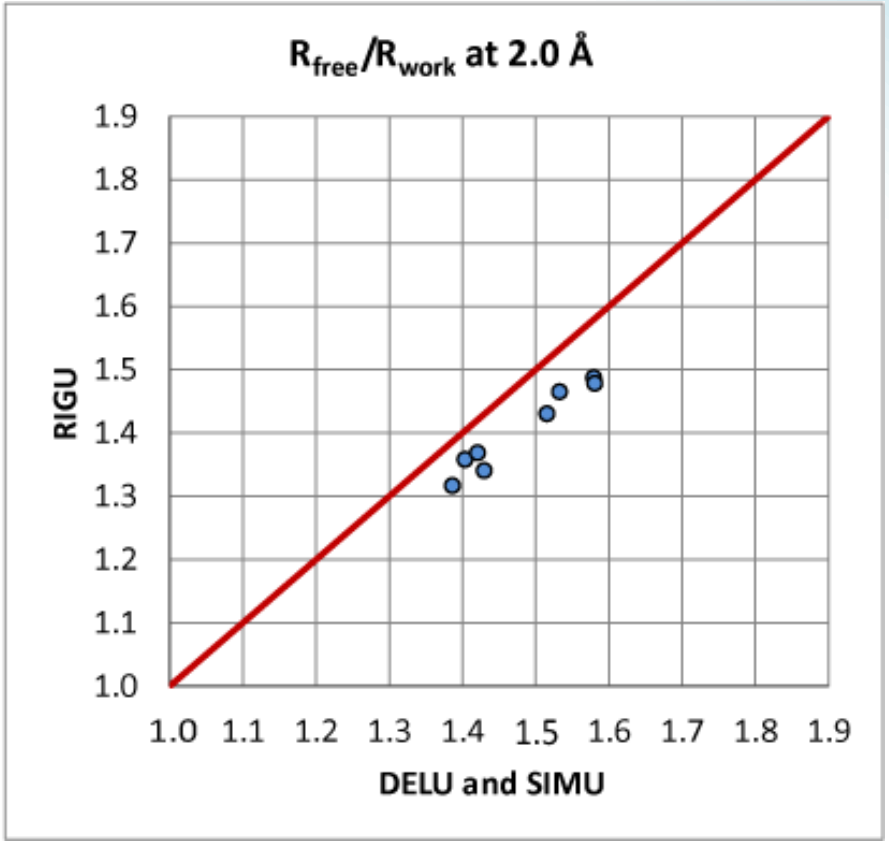
- 0.7 - 1.2 Å
- 55 - 331 residues
- minor components of disordered residues removed
- water molecules refined isotropically
- structures ‘shaken’ by random shifts (mean of 0.5 Å)

*** 1b0y, 1lu0, 1ok0, 1rqw, 1us0, 2cm5, 2fdn and 2vb1**

Tests

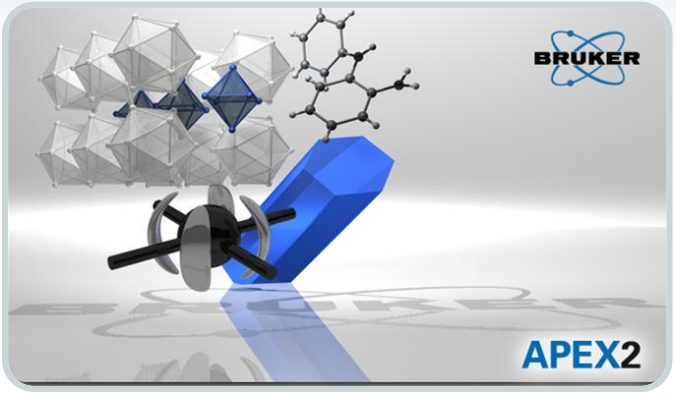
1.7 Å resolution





Using SHELXL-2013 with APEX2

APEX2 and SHELXL-2013



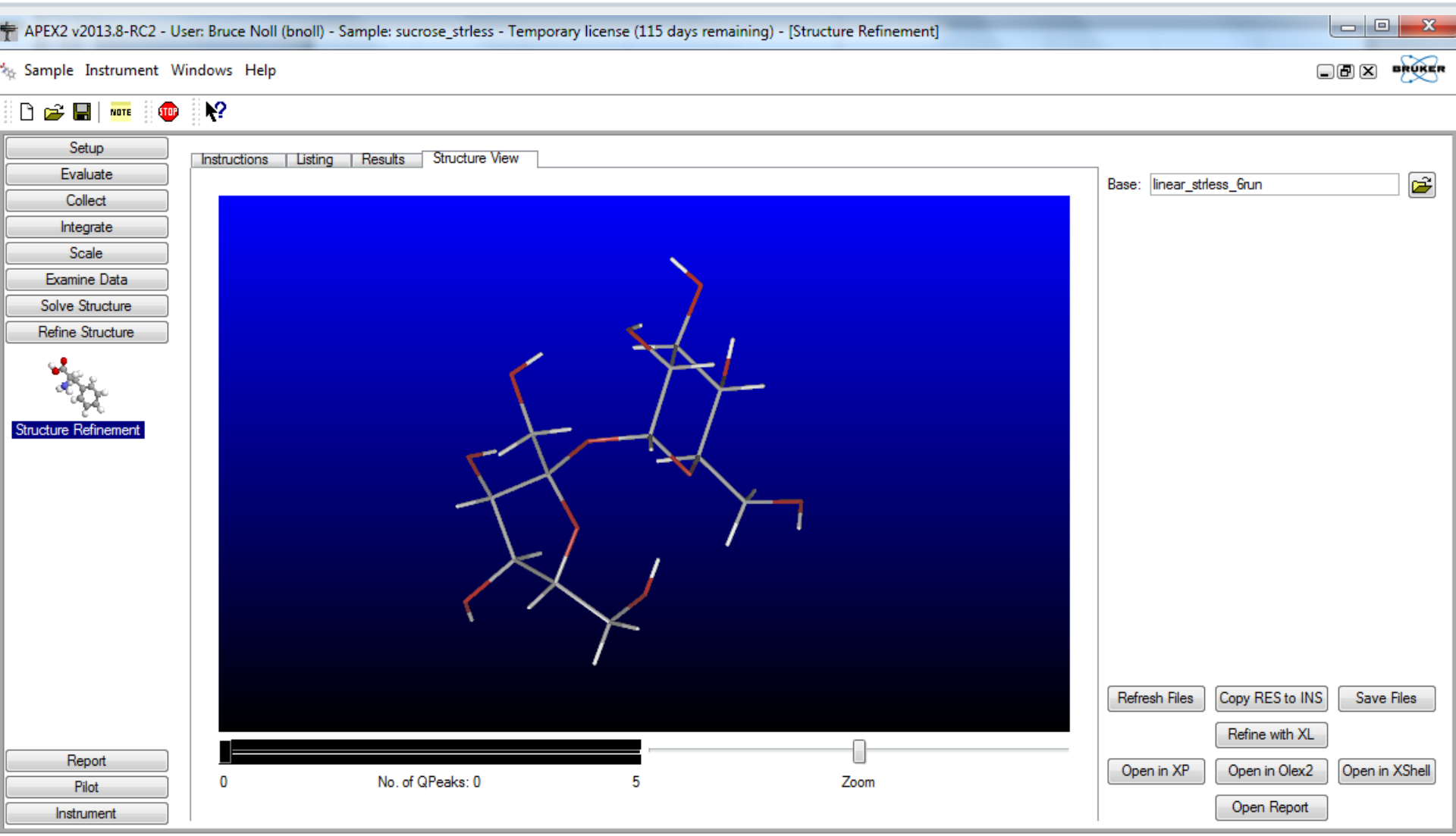

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+  SHELXL -  CRYSTAL STRUCTURE REFINEMENT  -   MULTI-CPU VERSION  +
+  Copyright(C) George M. Sheldrick 1993-2013     Version 2013/4  +
+  twin5                      started at 16:12:13 on 21-Aug-2013  +
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Command line parameters: twin5 -a50000 -b3000 -c624 -t4

-a sets the approximate maximum number of atoms including hydrogens.
-b sets the maximum number of full-matrix parameters (leave unchanged for
CGLS). For example -b9000 allows refinement of 1000 anisotropic atoms or
3000 with BLOC 1. For a 32-bit version, -b times the square root of the
number of threads should not exceed about 65500. -c sets the reflection
buffer size. This depends on the CPU cache size but will rarely need
changing. -t sets the number of threads, otherwise the multi-CPU version
sets this equal to the number of available CPUs. For optimal performance
on systems with hyperthreading, usually the hyperthreading should be
switched off or -t used to halve the number of threads; e.g. -t4 rather
than -t8 for an Intel i7 processor.

Running  4 threads on  4 processors
```

- SHELXL is engine underlying refinement in APEX2
- Structure Refinement plug-in allows easy interaction with SHELXL-2013
- Refinement instructions handled directly
- New CIF requirements met during refinement

Refinement

- All new commands can be used within Structure Refinement plug-in

The Structure Refinement Plug-In



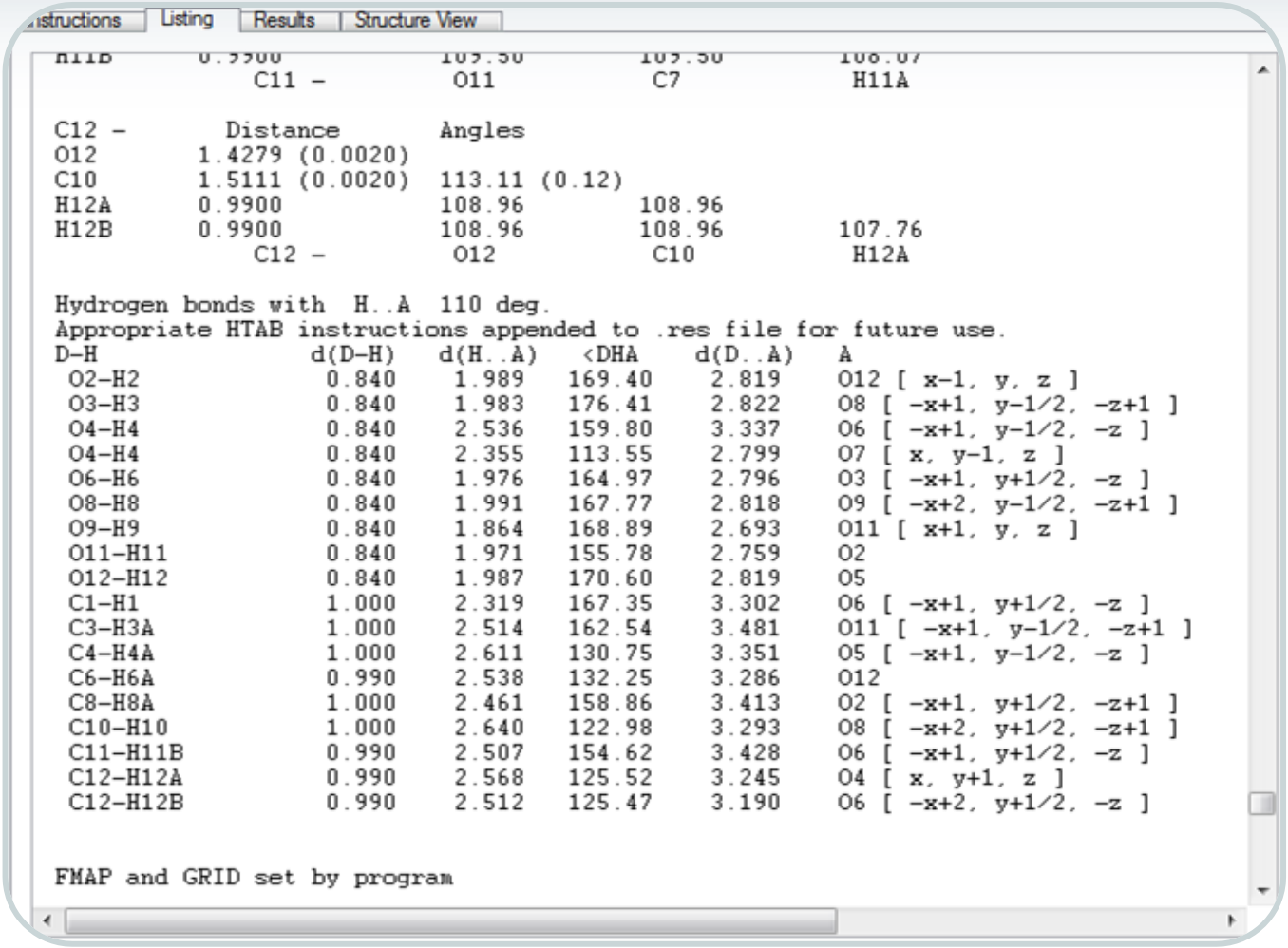
Hydrogen Bonding

Instructions | Listing | Results | Structure View

```
H12A  2    0.879936    0.724993    0.136234    11.00000   -1.20000
H12B  2    1.073165    0.709329    0.228599    11.00000   -1.20000
AFIX   0
HKLF 4

REM  linear_strless_6run in P2(1)
REM R1 =  0.0243 for    3452 Fo > 4sig(Fo)  and  0.0248 for all    3505 data
REM    216 parameters refined using      1 restraints

END

WGHT      0.0376      0.1521

REM Instructions for potential hydrogen bonds
EQIV $1 x-1, y, z
HTAB O2 O12_$1
EQIV $2 -x+1, y-1/2, -z+1
HTAB O3 O8_$2
EQIV $3 -x+1, y-1/2, -z
HTAB O4 O6_$3
EQIV $4 x, y-1, z
HTAB O4 O7_$4
EQIV $5 -x+1, y+1/2, -z
HTAB O6 O3_$5
EQIV $6 -x+2, y-1/2, -z+1
HTAB O8 O9_$6
EQIV $7 x+1, y, z
HTAB O9 O11_$7
HTAB O11 O2
HTAB O12 O5
HTAB C1 O6_$5
HTAB C3 O11_$2
HTAB C4 O5_$3
HTAB C6 O12
EQIV $8 -x+1, y+1/2, -z+1
HTAB C8 O2_$8
EQIV $9 -x+2, y+1/2, -z+1
HTAB C10 O8_$9
HTAB C11 O6_$5
EQIV $10 x, y+1, z
HTAB C12 O4_$10
EQIV $11 -x+2, y+1/2, -z
HTAB C12 O6_$11

REM Highest difference peak  0.319,  deepest hole -0.179,  1-sigma level  0.042
Q1    1   0.8675  0.5637  0.4638  11.00000  0.05    0.32
Q2    1   0.5377  0.5836  0.3823  11.00000  0.05    0.32
Q3    1   0.5013  0.0911  0.1765  11.00000  0.05    0.29
Q4    1   0.7535  0.1860  0.0860  11.00000  0.05    0.29
Q5    1   0.9127  0.6763  0.2660  11.00000  0.05    0.29
```

- Insert HTAB instruction
- List of possible hydrogen bonds automatically generated
- Review and paste into instructions
- Properly formatted for direct transfer to CIF file

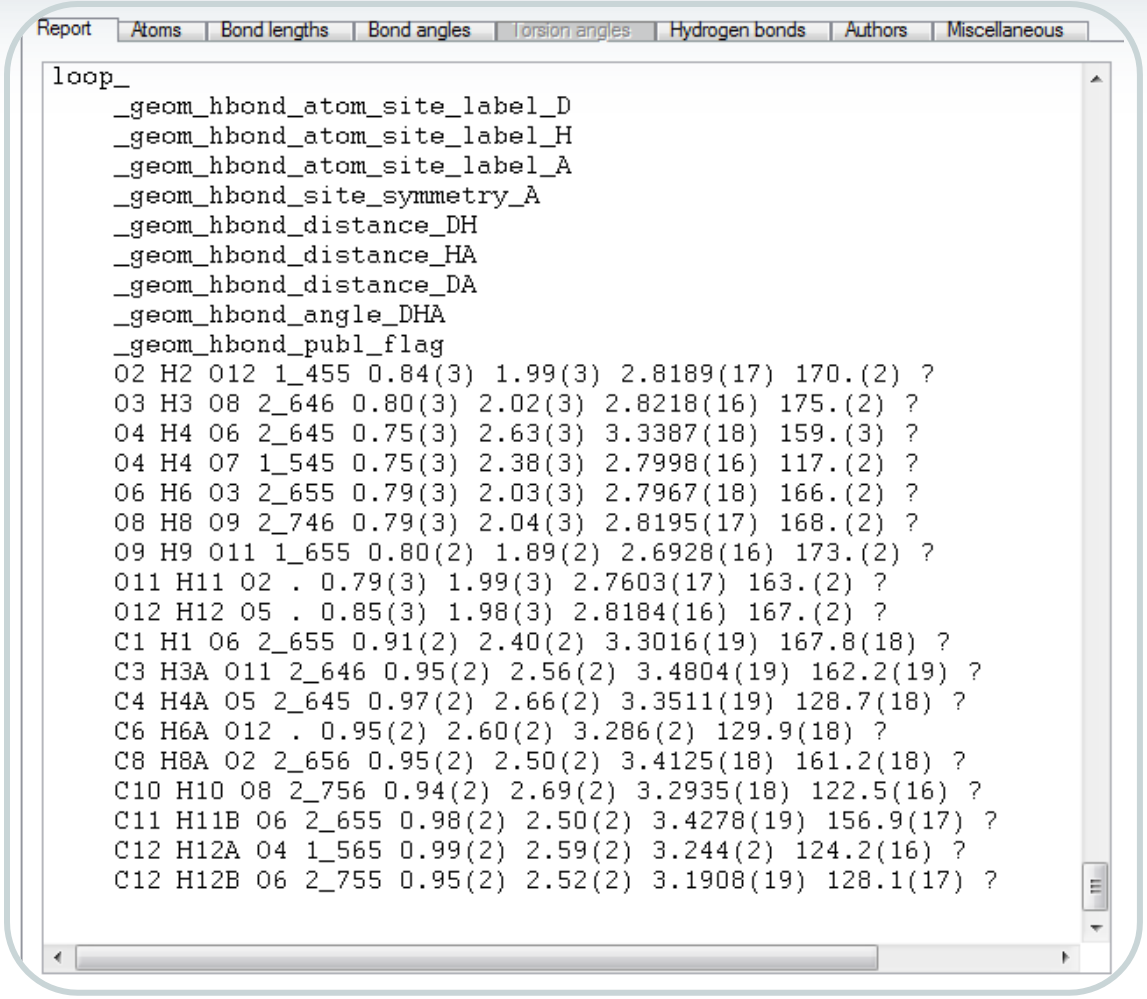
Hydrogen Bonds in .lst File



istructions | Listing | Results | Structure View

```
H11B      0.9900          109.50          109.50          108.07
              C11 -           O11             C7              H11A

C12 -       Distance        Angles
O12       1.4279 (0.0020)
C10       1.5111 (0.0020)   113.11 (0.12)
H12A      0.9900            108.96          108.96
H12B      0.9900            108.96          108.96          107.76
              C12 -           O12             C10             H12A

Hydrogen bonds with  H..A  110 deg.
Appropriate HTAB instructions appended to .res file for future use.
D-H                d(D-H)    d(H..A)    <DHA     d(D..A)    A
 O2-H2              0.840     1.989    169.40     2.819    O12 [ x-1, y, z ]
 O3-H3              0.840     1.983    176.41     2.822    O8 [ -x+1, y-1/2, -z+1 ]
 O4-H4              0.840     2.536    159.80     3.337    O6 [ -x+1, y-1/2, -z ]
 O4-H4              0.840     2.355    113.55     2.799    O7 [ x, y-1, z ]
 O6-H6              0.840     1.976    164.97     2.796    O3 [ -x+1, y+1/2, -z ]
 O8-H8              0.840     1.991    167.77     2.818    O9 [ -x+2, y-1/2, -z+1 ]
 O9-H9              0.840     1.864    168.89     2.693    O11 [ x+1, y, z ]
 O11-H11            0.840     1.971    155.78     2.759    O2
 O12-H12            0.840     1.987    170.60     2.819    O5
 C1-H1              1.000     2.319    167.35     3.302    O6 [ -x+1, y+1/2, -z ]
 C3-H3A             1.000     2.514    162.54     3.481    O11 [ -x+1, y-1/2, -z+1 ]
 C4-H4A             1.000     2.611    130.75     3.351    O5 [ -x+1, y-1/2, -z ]
 C6-H6A             0.990     2.538    132.25     3.286    O12
 C8-H8A             1.000     2.461    158.86     3.413    O2 [ -x+1, y+1/2, -z+1 ]
 C10-H10            1.000     2.640    122.98     3.293    O8 [ -x+2, y+1/2, -z+1 ]
 C11-H11B           0.990     2.507    154.62     3.428    O6 [ -x+1, y+1/2, -z ]
 C12-H12A           0.990     2.568    125.52     3.245    O4 [ x, y+1, z ]
 C12-H12B           0.990     2.512    125.47     3.190    O6 [ -x+2, y+1/2, -z ]


FMAP and GRID set by program
```

Creating Hydrogen Bond Table in CIF file



- CIF H-bonding table
  - "loop_" and headers generated
  - Data fields populated
- All automatic from instructions inserted to .ins file

CIF and SHEXL Files

PLAT005

PLAT005 Type_5 Check for refinement instruction file No 'refinement details' record was found. *Acta Cryst.* requires the inclusion of the last shelxl.res file (in case of a SHELXL or XL refinement) in the CIF embedded between records with semicolons in position 1, preceded by an '_iucr_refine_instructions_details' record.

Note: SHELXL2013 will automatically include the final .res as an embedded comment with the dataname '_shelx_res_file'.

- Include .res file and .hkl file to avoid this alert

The 2013 CIF File

- Notable Changes
  - Inclusion of refinement results
  - Inclusion of intensity data
- Benefits
  - Increases experimental transparency
  - SHELX users can easily review instructions, restraints, results
  - Repeat refinement after extracting files from CIF file
- Drawbacks
  - Including files increases complexity of CIF file
  - Including hkl file may increase file size by thousands of lines

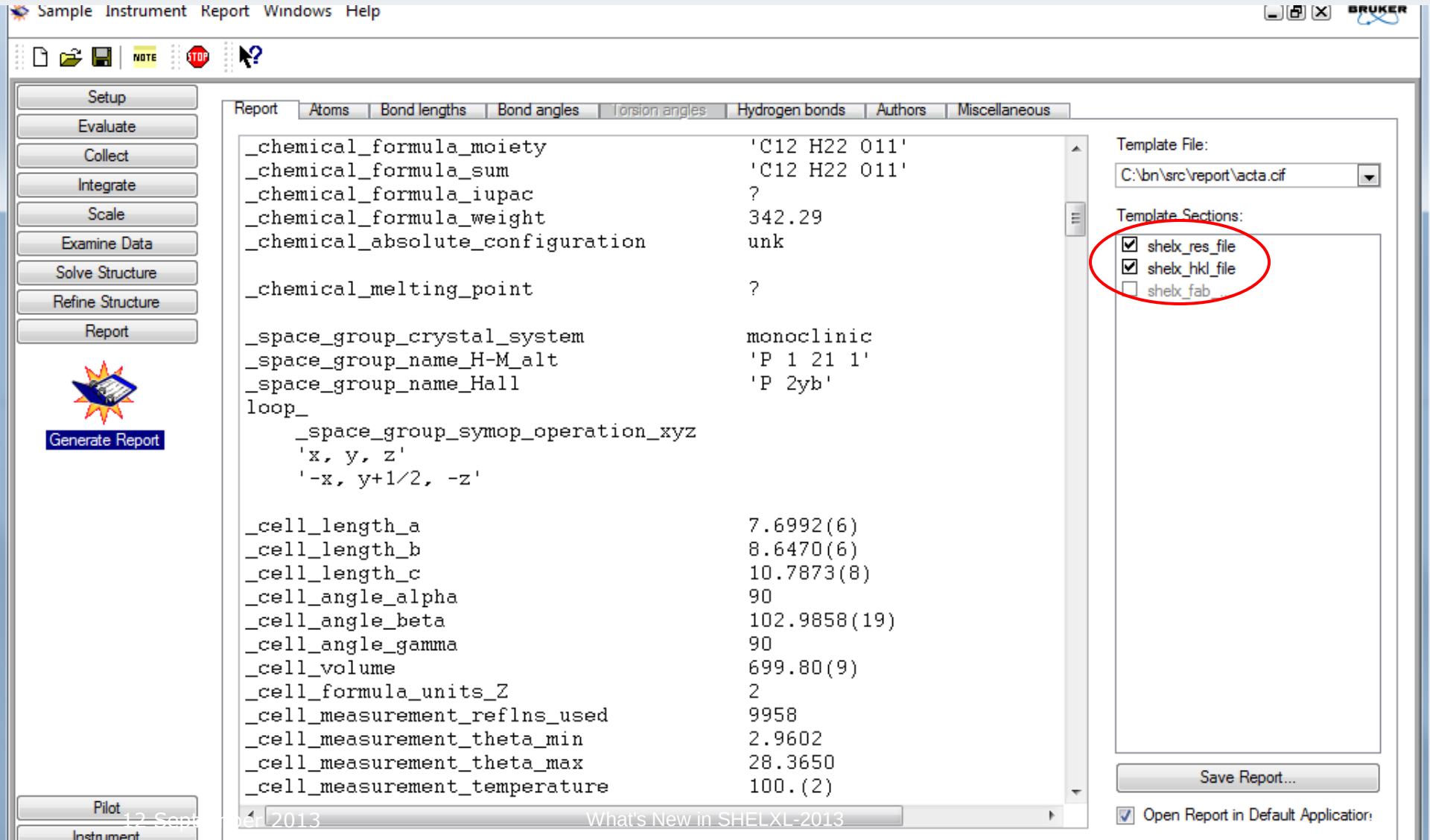
```
_shelx_res_file
;
TITL linear_strless_6run in P2(1)
CELL 0.71073   7.69920   8.64700  10.78730  90.0000 102.9858  90.0000
ZERR    2.00   0.00060   0.00060   0.00080   0.0000   0.0019   0.0000
LATT -1
SYMM -X, 0.5+Y, -Z
SFAC C  H  O
UNIT 24  44  22
REM Solution 1  R1  0.061,  Alpha= 0.0028  in P2(1)
REM Flack x= -0.224 ( 0.183 ) from Parsons' quotients
REM C12 O11
REM Instructions for potential hydrogen bonds
EQIV $1 x-1, y, z
HTAB O2 O12_$1
EQIV $2 -x+1, y-1/2, -z+1
HTAB O3 O8_$2
EQIV $3 -x+1, y-1/2, -z
HTAB O4 O6_$3
EQIV $4 x, y-1, z
HTAB O4 O7_$4
EQIV $5 -x+1, y+1/2, -z
HTAB O6 O3_$5
EQIV $6 -x+2, y-1/2, -z+1
HTAB O8 O9_$6
EQIV $7 x+1, y, z
HTAB O9 O11_$7
HTAB O11 O2
HTAB O12 O5
HTAB C1 O6_$5
HTAB C3 O11_$2
HTAB C4 O5_$3
HTAB C6 O12
EQIV $8 -x+1, y+1/2, -z+1
HTAB C8 O2_$8
EQIV $9 -x+2, y+1/2, -z+1
HTAB C10 O8_$9
HTAB C11 O6_$5
EQIV $10 x, y+1, z
HTAB C12 O4_$10
EQIV $11 -x+2, y+1/2, -z
HTAB C12 O6_$11
L.S. 10
acta
```

The 2013 CIF File

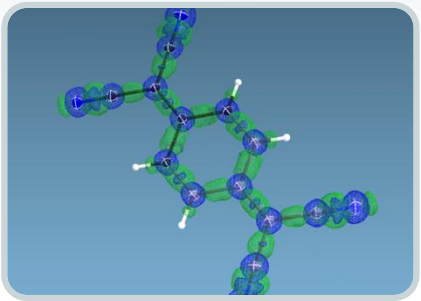
- Structure factors incorporated directly to CIF file as data under "_shelx_hkl_file"
- Checksum included at end of list to prevent tampering
- .res and .hkl files can be extracted from the CIF file using "shredCIF"

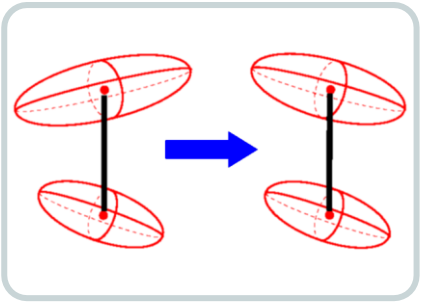
```
_shelx_hkl_file
;
   2   0   0   94.40    1.94
   2   0   0   99.26    2.11
   2   0   0   95.38    1.91
   2   0   0   96.59    1.89
   2   0   0   96.14    1.91
  -2   0   0   96.95    1.95
  -2   0   0   94.02    1.90
  -2   0   0   98.19    2.11
  -2   0   0   97.78    1.92
  -3   0   0  333.24    6.43
  -3   0   0  335.35    6.56
   3   0   0  331.67    7.17
   3   0   0  331.75    6.60
   3   0   0  339.17    6.42
   3   0   0  327.17    6.55
   3   0   0  317.59    6.60
   3   0   0  337.35    6.42
  -3   0   0  340.45    7.17
  -3   0   0  339.55    6.41
  -4   0   0   46.65    1.06
   4   0   0   46.32    1.08
   4   0   0   45.77    1.00
  -4   0   0   44.78    1.06
  -4   0   0   47.76    1.08
  -4   0   0   45.69    1.05
   4   0   0   46.54    1.08
   4   0   0   47.07    1.00
   0   0   0    0.00    0.00
;
_shelx_hkl_checksum                20093
```

Report Generator and CIF Template



What's New in SHELXL-2013?





- Increased ability to handle difficult structures
  - RIGU restraint
  - XNPD constraint
  - improved absolute structure determination
- Additional tools for refinement
  - neutron data facilities
  - faster refinement with multi-processor usage
- Improvements in concert with CIF changes
  - SHELX files embedded for re-refinement
  - compliance with core-CIF version 2.4.3.

Conclusion

SHEXL-2013 continues the power and flexibility of SHEXL-97 and its predecessors.

Any questions?

Please type any questions you may have for our speakers in the Q&A panel and click Send.

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Webinar	Content
Apr 02, 2013 **Fast, Intuitive Structure Determination II: Crystal Indexing and Data Collection Strategies**	Attend this one-hour webinar to learn skills for crystal indexing and data collection. Dr. Bruce Noll will cover the APEX2 tools that can be used to select reflections and sort them into arrays to facilitate indexing routine, twin and modulated structures. He will also examine the diffraction behavior of the sample to determine the best data collection parameters. Register now
Feb 26, 2013 **Advanced Crystallography: Data Collection and Data Reduction Techniques for Modulated Structures**	Drs. Michael Ruf and Charles Campana give a one-hour presentation demonstrating the steps required to collect and process data for modulated structures. Specific topics include: how to recognize modulated structures; introduction to q-vectors; APEX2 software tools; preparation of files for JANA2006; and examples of the solution of modulated structures from single-crystal diffraction data. View recording Download slides
Dec 05, 2012 **PROTEUM2 and Foreign Frame Formats**	View this 45-minute webinar to learn about Bruker's PROTEUM software, a suite of crystallographic data integration and reduction tools for macromolecules. Dr. Matt Benning and Dr. Michael Ruf will discuss how to reduce data from various detectors and show results from synchrotron beamlines. View recording Download slides
Nov 13, 2012 **Advanced Crystallography: Refinement of Disordered Structures**	Dr. Charles Campana gives a one-hour presentation demonstrating the steps required to refine disordered crystal structures. Along with specific examples, topics covered include SHELXL, SHELXTL, free variables, PART n and –n instructions, constraints vs restraints, and advanced refinement instructions. View recording Download slides
Dec 06, 2011 **High-Pressure Crystallography**	Dr. Francesca Fabbiani of Georg-August-Universität Göttingen takes you through the steps for performing a high-pressure single-crystal X-ray diffraction experiment with a diamond-anvil cell (DAC). You will learn DAC loading techniques and useful strategies for data collection, data reduction, and structure refinement. View recording Download slides
Oct 13, 2011 **Advanced Crystallography – Publication of Crystal Structures**	Publication of crystal structures is often a researcher's least favorite task. This 90-min webinar will help. It describes the steps required to prepare crystal structures for publication in chemical and crystallographic journals, including collection of high-quality intensity data, common refinement problems, data evaluation, error analysis, preparation of CIF files, and the use of CIF-checking programs. View recording Download slides
Jun 22, 2011 **CMOS: The Next Generation in X-ray Detector Technology**	CCDs have long been one of the most important detector technologies for X-ray crystallography. Recently, however, new detectors based on CMOS technology have begun to supplant CCDs. View this webinar to learn about Bruker AXS' new X-ray detector based on CMOS technology, the PHOTON 100. View recording Download slides
May 03, 2011 **Using APEX2 to Analyze Twinned Crystals**	Twinned crystals are common occurrences in many laboratories and pose special challenges in structure solution. View this 76-minute webinar to learn how to visualize, index, integrate, scale, solve and refine structure data from twinned crystals with the APEX2 software suite. (Note: playback begins at 14:00 minutes into the 1:30:20 hour presentation.) View recording Download slides
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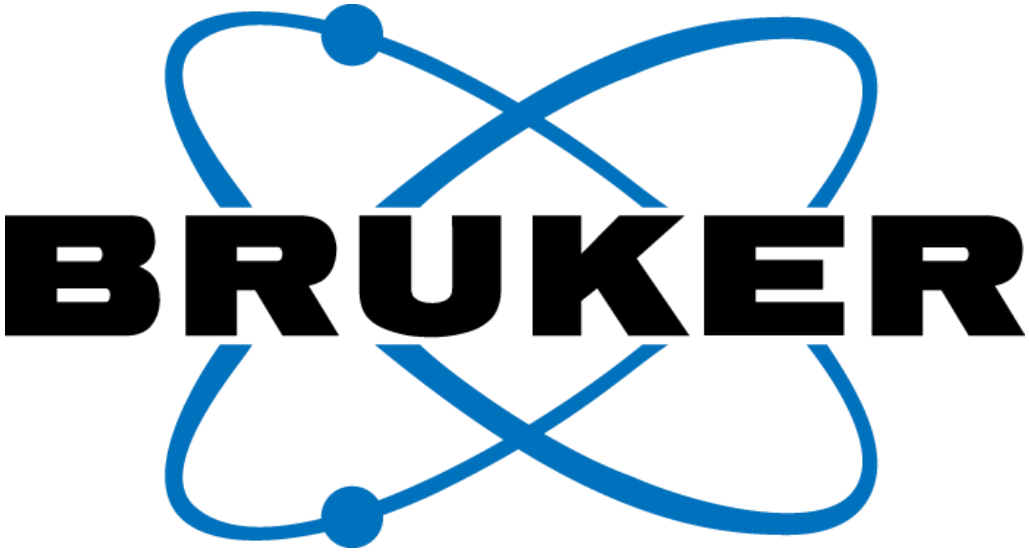

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