AIC International Crystallography School 2019

CRYSTALLOGRAPHIC INFORMATION FIESTA

Naples, Italy
30 August - 3 September 2019

PUBLICATION: PREPARING SMALL-MOLECULE STRUCTURE REPORTS FOR IUCr JOURNALS

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https://scvsa-servizi.campusnet.unipr.it/do/docenti.pl/Alias?chiara.massera#profilo

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IUCr J — IUCrJ
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https://journals.iucr.org/

The «must have» of a crystal structure

How to prepare a structure report

Software and tools – simplify your life!

OUTLINE

https://journals.iucr.org/e/services/cif/reqditems.html

https://journals.iucr.org/e/services/cif/reqdata.html

http://journals.iucr.org/services/cif/checking/platon_tests.html

File check.def - https://www.platonsoft.nl/platon/pl000601.html

MUST HAVE

RESOLUTION

The $theta_{max}$ of measured reflections should be such that sin $theta_{max}/\lambda$ exceeds 0.6 $Å^{-1}$ (*i.e.* $theta_{max}$ > 25° for Mo $K\alpha$; $theta_{max}$ > 67° for Cu $K\alpha$).

It is expected that all possible unique reflections out to at least the specified minimum limits are measured.

Alert level A

THETM01 ALERT 3 A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta max)/wavelength = 0.5401

Wavelength=1.54178 **θ_{max} = 56.37**

MUST HAVE

http://journals.iucr.org/services/cif/checking/THETM_01.html

CALCULATE

S = SIN [_diffrn_reflns_theta_max] / _diffrn_radiation_wavelength

TEST

IF S < 0.55 issue **ALERT** A

```
"Alert A The value of sine(theta_max)/wavelength is less than 0.550"
```

< 0.575 issue **ALERT** B

```
"Alert B The value of sine(theta_max)/wavelength is less than 0.575"
```

< 0.59 issue **ALERT** C

```
"Alert C The value of sine(theta_max)/wavelength is less than 0.590"
```

MUST HAVE

COMPLETENESS

_diffrn_measured_fraction_theta_max

This is the fraction of unique (symmetry-independent) reflections measured out to _diffrn_reflns_theta_max. Ideally, this should be as close to 1.0 as possible.

_diffrn_measured_fraction_theta_full

Fraction of unique (symmetry-independent) reflections measured out to **_diffrn_reflns_theta_full.** This has to be close to 1.0

$theta_{full}$ is the diffractometer angle at which the measured reflection count is close to complete.

MUST HAVE

COMPLETENESS

tma071.cif - enCIFer

File Edit Search Tools Help

Blocks: 1

```
_diffrn_detector_area_resol_mean  ?
_diffrn_reflns_number             34742
_diffrn_reflns_av_unetI/netI      0.0974
_diffrn_reflns_av_R_equivalents   0.0579
_diffrn_reflns_limit_h_min        -13
_diffrn_reflns_limit_h_max        12
_diffrn_reflns_limit_k_min        -19
_diffrn_reflns_limit_k_max        19
_diffrn_reflns_limit_l_min        -35
_diffrn_reflns_limit_l_max        36
_diffrn_reflns_theta_min          1.794
_diffrn_reflns_theta_max          25.923
_diffrn_reflns_theta_full         24.835
_diffrn_measured_fraction_theta_max   0.854
_diffrn_measured_fraction_theta_full  0.883
_diffrn_reflns_Laue_measured_fraction_max    0.854
_diffrn_reflns_Laue_measured_fraction_full   0.883
_diffrn_reflns_point_group_measured_fraction_max   0.854
_diffrn_reflns_point_group_measured_fraction_full  0.883
_reflns_number_total              20813
_reflns_number_gt                 12492
_reflns_threshold_expression      'I > 2\s(I)'
_reflns_Friedel_coverage          0.000
_reflns_Friedel_fraction_max      .
_reflns_Friedel_fraction_full     .
```

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

Bond precision: C-C = 0.0103 A Wavelength=0.70000

Cell: a=12.472(2) b=16.173(2) c=29.790(1)
alpha=90.927(1) beta=93.632(3) gamma=95.386(2)
Temperature: 100 K

	Calculated	Reported
Volume	5968.9(12)	5968.9(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C128 H148 N8 O16, C6 H12	(C128 H152 O16 N8), (C6 H12)
Sum formula	C134 H160 N8 O16	C134 H164 N8 O16
Mr	2138.71	2142.72
Dx,g cm-3	1.190	1.192
Z	2	2
Mu (mm-1)	0.074	0.076
F000	2296.0	2304.0
F000'	2296.89	
h,k,lmax	15,20,37	13,19,36
Nref	24375	20813
Tmin,Tmax	0.991,0.994	0.842,1.000
Tmin'	0.991	

Correction method= # Reported T Limits: Tmin=0.842 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.854 Theta(max)= 25.923

R(reflections)= 0.1423(12492) wR2(reflections)= 0.5205(20813)

S = 1.008 Npar= 1432

Data completeness= 1.48/0.86

MUST HAVE

COMPLETENESS

Alert level A

PLAT029 ALERT 3 A	_diffrn_measured_fraction_theta_full value Low .	0.883 Why?
PLAT084 ALERT 3 A	High wR2 Value (i.e. > 0.25)	0.52 Report
PLAT201 ALERT 2 A	Isotropic non-H Atoms in Main Residue(s)	23 Report
	C12B C13B C23A C24A C25A C26A	etc.
PLAT360 ALERT 2 A	Short C(sp3)-C(sp3) Bond C12A - C13A .	1.22 Ang.
PLAT360 ALERT 2 A	Short C(sp3)-C(sp3) Bond C12B - C13B .	1.17 Ang.
PLAT360 ALERT 2 A	Short C(sp3)-C(sp3) Bond C29D - C30D .	1.21 Ang.
PLAT410 ALERT 2 A	Short Intra H...H Contact H27O ..H26S .	1.75 Ang.
	x,y,z =	1_555 Check

Alert A: $\leq$ 0.0939

0.94 < Alert B < 0.959

0.96 < Alert C < 0.979

No Alert: $\geq$ 0.98

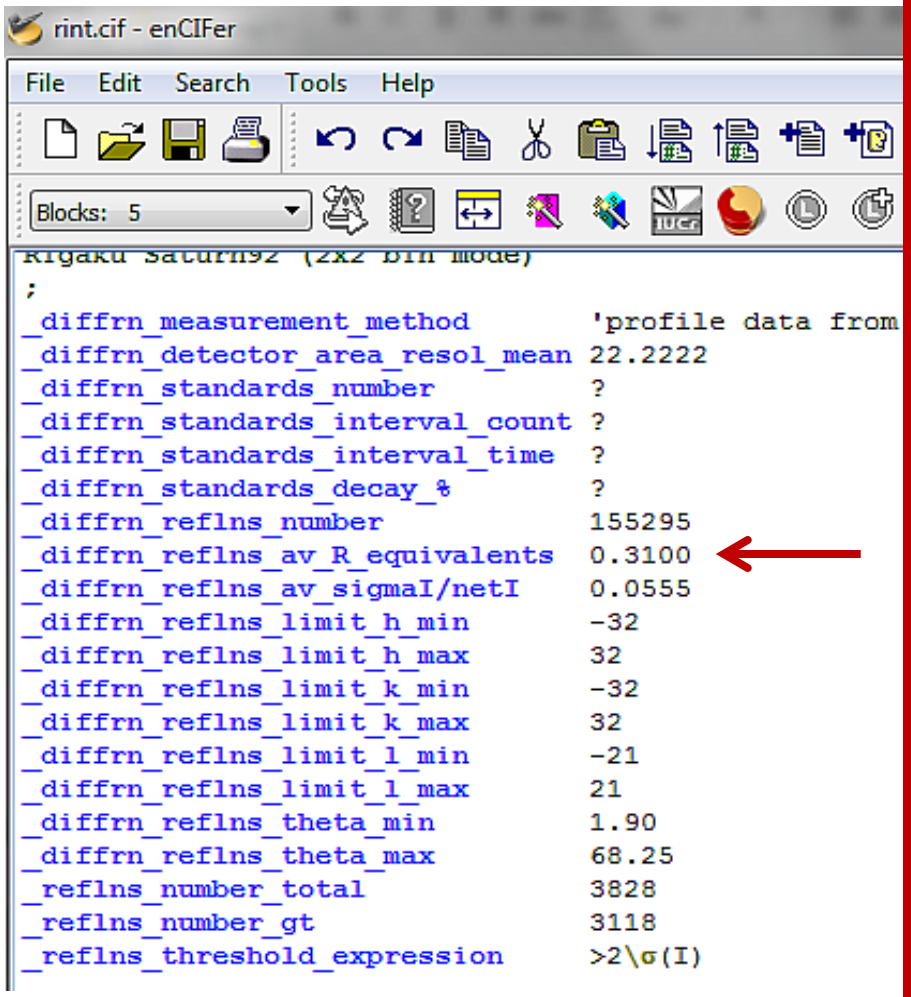
MUST HAVE

EQUIVALENT REFLECTIONS

_diffrn_reflns_av_R_equivalents

Sufficient symmetry-equivalent reflections must be measured to provide a good estimate of the intensity reproducibility.

The value of ***R_{int} should normally be considerably less than 0.10-0.12*** and in the order of magnitude of the reported R-values



MUST HAVE

EQUIVALENT REFLECTIONS

Alert level A

RINTA01 ALERT 3 A The value of Rint is greater than 0.25
Rint given 0.310

http://journals.iucr.org/services/cif/checking/RINTA_01.html

PROC-NAME: **RINTA01** Type_3

PURPOSE: To check that _diffrn_reflns_av_R_equivalents is within expected limits.

PROCEDURE:
TEST
IF _diffrn_reflns_av_R_equivalents > 0.20 issue **ALERT** A
"Alert A The value of Rint is greater than 0.20"
> 0.15 issue **ALERT** B
"Alert B The value of Rint is greater than 0.15"
> 0.10 issue **ALERT** C
"Alert C The value of Rint is greater than 0.10"
< 0.0 issue **ALERT** A
"Alert A The value of Rint is less than 0.0"

MUST HAVE

FINAL REFINEMENT

_refine_ls_shift/su_max

This is the largest ratio of the parameter shift to standard uncertainty after the final round of refinement and is typically within ±0.01 if sufficient least-squares refinement cycles have been employed. A value above ±0.05 is considered unusual and values beyond ±0.1 are a sign of incomplete refinement, unaccounted-for disorder or high correlation between parameters that should be constrained.

journals.iucr.org/services/cif/checking/SHFSU_01.html

PROC-NAME: SHFSU01 Type_2

PURPOSE: To check that _refine_ls_shift/su_max is within expected limits.

PROCEDURE:
TEST
IF |_refine_ls_shift/su_max| > 0.20 issue **ALERT** A
"Alert A The absolute value of parameter shift to su ratio > 0.20"
> 0.10 issue **ALERT** B
"Alert B The absolute value of parameter shift to su ratio > 0.10"
> 0.05 issue **ALERT** C
"Alert C The absolute value of parameter shift to su ratio > 0.05"

MUST HAVE

FINAL REFINEMENT

```
Running  4 threads on  4 processors

Read instructions and data
Data:   20927 unique,      0 suppressed   R(int) = 0.0519   R(sigma) = 0.0606
Systematic absence violations:    0    Bad equivalents:    3
wR2 = 0.1388 before cycle   1 for   20927 data and   1095 /   1095 parameters
GooF = S =     1.014;     Restrained GooF =      1.015 for      15 restraints
Mean shift/esd =   0.024  Maximum =    -0.184 for  U11 La1        at 14:41:34
Max. shift = 0.009 A for H8W      Max. dU = 0.001 for O5D_b
wR2 = 0.1388 before cycle   2 for   20927 data and   1095 /   1095 parameters
GooF = S =     1.014;     Restrained GooF =      1.015 for      15 restraints
Mean shift/esd =   0.009  Maximum =    -0.064 for  U11 La1        at 14:41:36
Max. shift = 0.005 A for H8SB      Max. dU = 0.000 for H7W
wR2 = 0.1389 before cycle   3 for   20927 data and   1095 /   1095 parameters
GooF = S =     1.015;     Restrained GooF =      1.015 for      15 restraints
Mean shift/esd =   0.001  Maximum =     0.042 for   y  H16W       at 14:41:38
Max. shift = 0.002 A for H17W      Max. dU = 0.000 for O5D_b
wR2 = 0.1389 before cycle   4 for   20927 data and   1095 /   1095 parameters
GooF = S =     1.015;     Restrained GooF =      1.015 for      15 restraints
Mean shift/esd =   0.001  Maximum =     0.036 for   y  H16W       at 14:41:40
Max. shift = 0.002 A for H17W      Max. dU = 0.000 for H7W
wR2 = 0.1389 before cycle   5 for   20927 data and      0 /   1095 parameters
GooF = S =     1.015;     Restrained GooF =      1.015 for      15 restraints
R1 =  0.0498 for   16270 Fo > 4sig(Fo)  and  0.0719 for all   20927 data
wR2 =  0.1389,  GooF = S =   1.015,  Restrained GooF =    1.015  for all data
** Warning:     6  atoms may be split and     0  atoms NPD **
R1 =  0.0699 for  20927 unique reflections after merging for Fourier
Highest peak    2.06  at  0.8380  0.6636  0.1621  [  0.54 A from O5D ]
Deepest hole   -1.48  at  0.0262  0.6149  0.1533  [  0.50 A from O5H ]

+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+  shelx         finished at 14:41:41   Total elapsed time:      9.39 secs  +
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

MUST HAVE

FINAL REFINEMENT

_refine_diff_density_min

_refine_diff_density_max

These values are expected to be small, especially for light-atom structures. If their magnitudes are such that a validation alert is generated, the label and the distance of the closest atom site should be reported in _publ_section_exptl_refinement.

```
_refine_diff_density_max    2.063
_refine_diff_density_min   -1.480
_refine_diff_density_rms    0.099
```

```
R1 =  0.0699 for  20927 unique reflections after merging for Fourier
Highest peak    2.06  at  0.8380  0.6636  0.1621  [  0.54 A from O5D ]
Deepest hole   -1.48  at  0.0262  0.6149  0.1533  [  0.50 A from O5H ]

++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+  shelx         finished at 14:41:41   Total elapsed time:      9.39 secs  +
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

http://journals.iucr.org/services/cif/checking/PLAT097.html

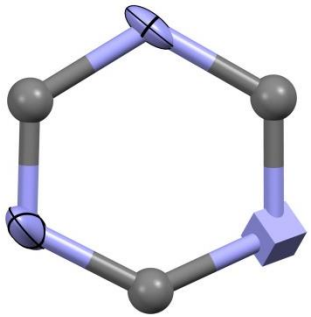
http://journals.iucr.org/services/cif/checking/PLAT098.html

MUST HAVE

FINAL REFINEMENT

_atom_site_aniso_U_

Checks will be made for non-positive definite anisotropic atomic displacement parameters (ADPs).



PLAT_211 Test for NPD ADP's in main residue(s) **ALERT A**

PLAT_212 Test for NPD ADP's in small moieties (solvent/anions) **ALERT B**

MUST HAVE

FINAL REFINEMENT

wR2 - in general it has a value twice of that of R1. Significantly larger values usually indicate a poor refinement model. Also check for unaccounted twinning.

http://journals.iucr.org/services/cif/checking/PLAT084.html

Alert level A

PLAT029 ALERT 3 A	_diffrn_measured_fraction_theta_full value Low .	0.883 Why?
PLAT084 ALERT 3 A	High wR2 Value (i.e. > 0.25)	0.52 Report
PLAT201 ALERT 2 A	Isotropic non-H Atoms in Main Residue(s)	23 Report
	C12B C13B C23A C24A C25A C26A	etc.
PLAT360 ALERT 2 A	Short C(sp3)-C(sp3) Bond C12A - C13A .	1.22 Ang.
PLAT360 ALERT 2 A	Short C(sp3)-C(sp3) Bond C12B - C13B .	1.17 Ang.
PLAT360 ALERT 2 A	Short C(sp3)-C(sp3) Bond C29D - C30D .	1.21 Ang.
PLAT410 ALERT 2 A	Short Intra H...H Contact H27O ..H26S .	1.75 Ang.
	x,y,z =	1_555 Check

0.25 **0.35** **0.45**

MUST HAVE

ABSOLUTE STRUCTURE

_refine_ls_abs_structure_details

This item should describe the method applied, with a literature citation if necessary, and the number of Friedel pairs used in the determination of the absolute structure parameter. Absolute structure is relevant in any non-centrosymmetric space group.

- Flack & Bernardinelli [*Acta Cryst*. (1999), A**55**, 908-915 ; *J. Appl. Cryst*. (2000), **33**, 1143-1148]
- Flack, Sadki, Thompson & Watkin [*Acta Cryst.* (2011), A**67**, 21-34]
- Jones [*Acta Cryst*. (1986), A**42**, 57]
- Hooft *et al.* [*J. Appl. Cryst.* (2008), **41**, 96-103; *J. Appl. Cryst.* (2010), **43**, 665-668]
- Parsons & Flack [*Acta Cryst*. (2004), A**60**, s61].

MUST HAVE

ABSOLUTE STRUCTURE

journals.iucr.org/services/cif/checking/STRVA_01.html

IF FLACK > 0.7 issue **ALERT** C
"Alert C Chirality of atom sites is inverted?"

IF FLACK > 0.3 ***AND*** FLACK < 0.7 issue **ALERT** C
"Alert C Flack test results are ambiguous."

IF FLACK < -0.2 issue **ALERT** C
"Alert C Flack parameter is too small.

IF SFLACK > 0.5 issue **ALERT** C
"Alert C Flack test results are meaningless."

MUST HAVE

ABSOLUTE STRUCTURE

journals.iucr.org/services/cif/checking/STRVA_01.html

Absolute structure parameter -0.4 (4)

"As a result of the unrealistic value obtained for the Flack absolute structure parameter [-0.4 (4) for 1097 quotients; Parsons et al., 2013], the absolute configuration of the pyranose ring system (2R,3S,4R,5R) was assigned on the basis of the known configuration for the starting compound d-glucose"

Acta Cryst. (2019). E**75**, 1096-1101

MUST HAVE

SQUEEZE

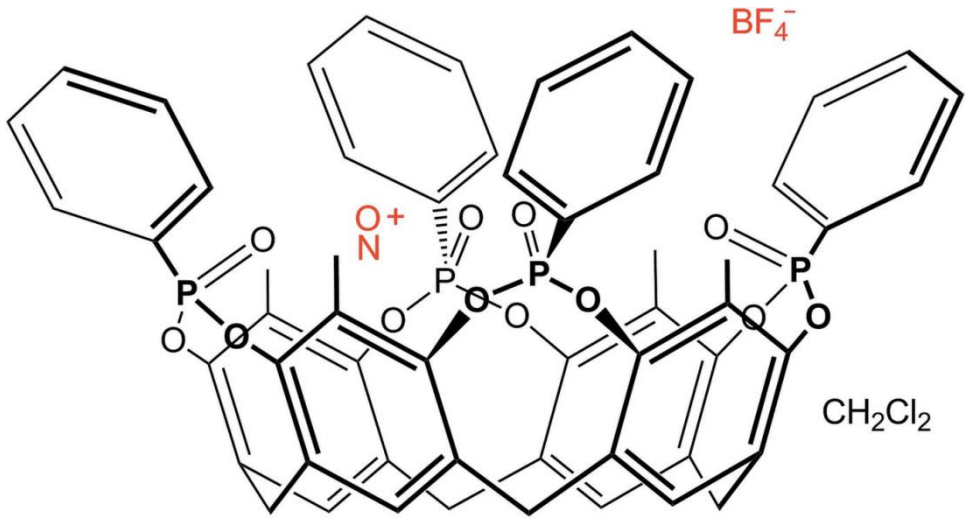
http://www.cryst.chem.uu.nl/spek/platon/pl000303.html

- the chemical formula should contain those parts that were removed with SQUEEZE (state explicitly if the solvent is unknown and the formula etc. does not include it)

- details of the SQUEEZE procedure to be reported in the 'Refinement section'

MUST HAVE

SQUEEZE



As a result of severe disorder, the CH_2Cl_2 solvent could not be sensibly modelled in terms of atomic sites, and was treated using the *PLATON* SQUEEZE procedure (Spek, 2015); the solvent contribution to the diffraction pattern was removed and modified F_o^2 written to a new HKL file. The number of electrons corresponding to the solvent molecules were included in the formula, formula weight, calculated density, μ and $F(000)$.

Acta Cryst. (2017). E**73**, 1801-1805

MUST HAVE

SQUEEZE

su5400.cif - enCIFer

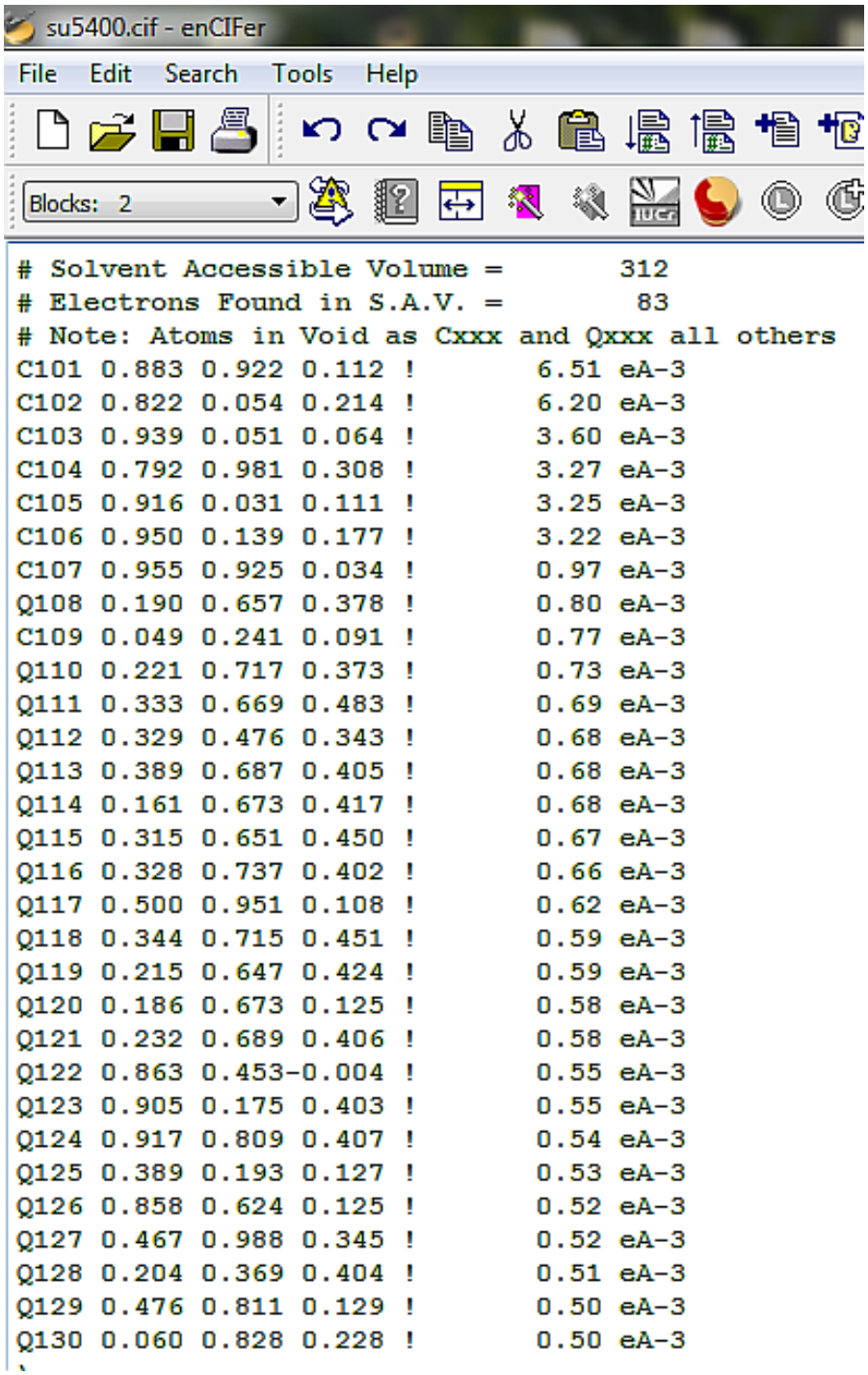
File Edit Search Tools Help

Blocks: 2

```
;
_chemical_name_common                ?
_chemical_formula_moiety              'C56 H44 P4 O12, N O +, B F4 -, (C H2 Cl2)'
_chemical_formula_sum                'C57 H46 B Cl2 F4 N O13 P4'
_chemical_formula_iupac               'C56 H44 P4 O12, N O +, B F4 -, C H2 Cl2'
_chemical_formula_weight              1234.54
```

```
_exptl_special_details
;
The calculated molar mass, density and absorption coefficient include
two disordered dichloromethane  molecules
per cell which do not appear in
the final files because of the  refinements
carried out with data subjected to SQUEEZE.
;
```

MUST HAVE


su5400.cif - enCIFer
File Edit Search Tools Help
Blocks: 2
Solvent Accessible Volume = 312
Electrons Found in S.A.V. = 83
Note: Atoms in Void as Cxxx and Qxxx all others
C101 0.883 0.922 0.112 ! 6.51 eA-3
C102 0.822 0.054 0.214 ! 6.20 eA-3
C103 0.939 0.051 0.064 ! 3.60 eA-3
C104 0.792 0.981 0.308 ! 3.27 eA-3
C105 0.916 0.031 0.111 ! 3.25 eA-3
C106 0.950 0.139 0.177 ! 3.22 eA-3
C107 0.955 0.925 0.034 ! 0.97 eA-3
Q108 0.190 0.657 0.378 ! 0.80 eA-3
C109 0.049 0.241 0.091 ! 0.77 eA-3
Q110 0.221 0.717 0.373 ! 0.73 eA-3
Q111 0.333 0.669 0.483 ! 0.69 eA-3
Q112 0.329 0.476 0.343 ! 0.68 eA-3
Q113 0.389 0.687 0.405 ! 0.68 eA-3
Q114 0.161 0.673 0.417 ! 0.68 eA-3
Q115 0.315 0.651 0.450 ! 0.67 eA-3
Q116 0.328 0.737 0.402 ! 0.66 eA-3
Q117 0.500 0.951 0.108 ! 0.62 eA-3
Q118 0.344 0.715 0.451 ! 0.59 eA-3
Q119 0.215 0.647 0.424 ! 0.59 eA-3
Q120 0.186 0.673 0.125 ! 0.58 eA-3
Q121 0.232 0.689 0.406 ! 0.58 eA-3
Q122 0.863 0.453-0.004 ! 0.55 eA-3
Q123 0.905 0.175 0.403 ! 0.55 eA-3
Q124 0.917 0.809 0.407 ! 0.54 eA-3
Q125 0.389 0.193 0.127 ! 0.53 eA-3
Q126 0.858 0.624 0.125 ! 0.52 eA-3
Q127 0.467 0.988 0.345 ! 0.52 eA-3
Q128 0.204 0.369 0.404 ! 0.51 eA-3
Q129 0.476 0.811 0.129 ! 0.50 eA-3
Q130 0.060 0.828 0.228 ! 0.50 eA-3

MUST HAVE

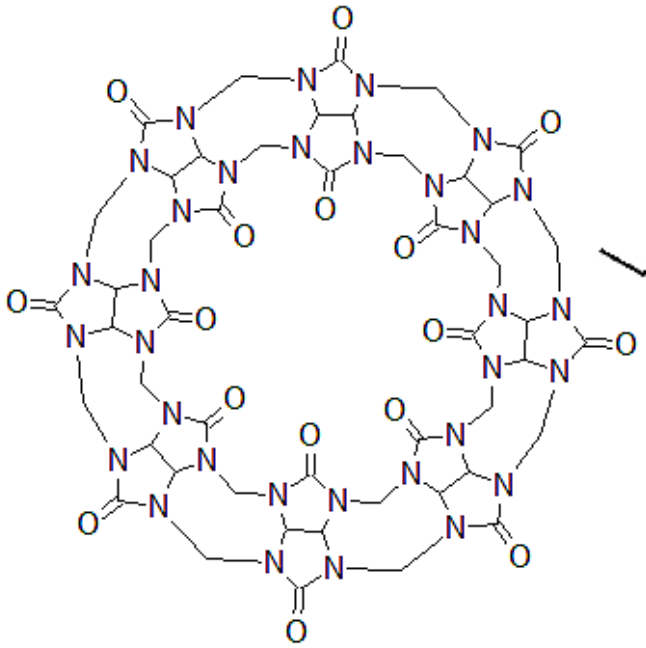
SHELXL

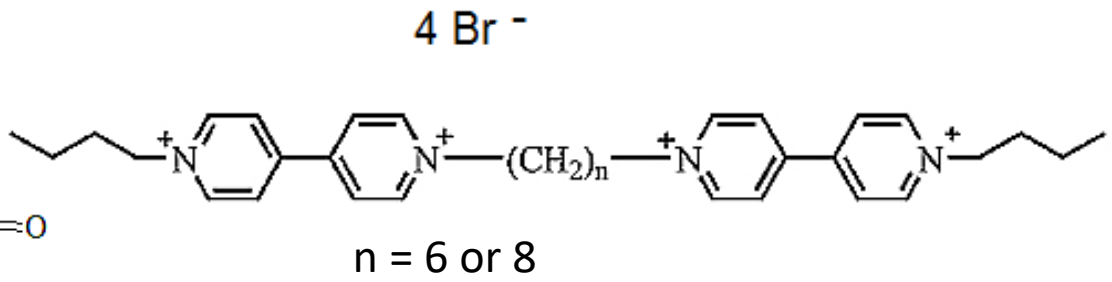
Authors should use the latest version of SHELXL. They should register at the SHELX Website http://shelx.uni-ac.gwdg.de/SHELX/register.php and download the latest version of the various programs.

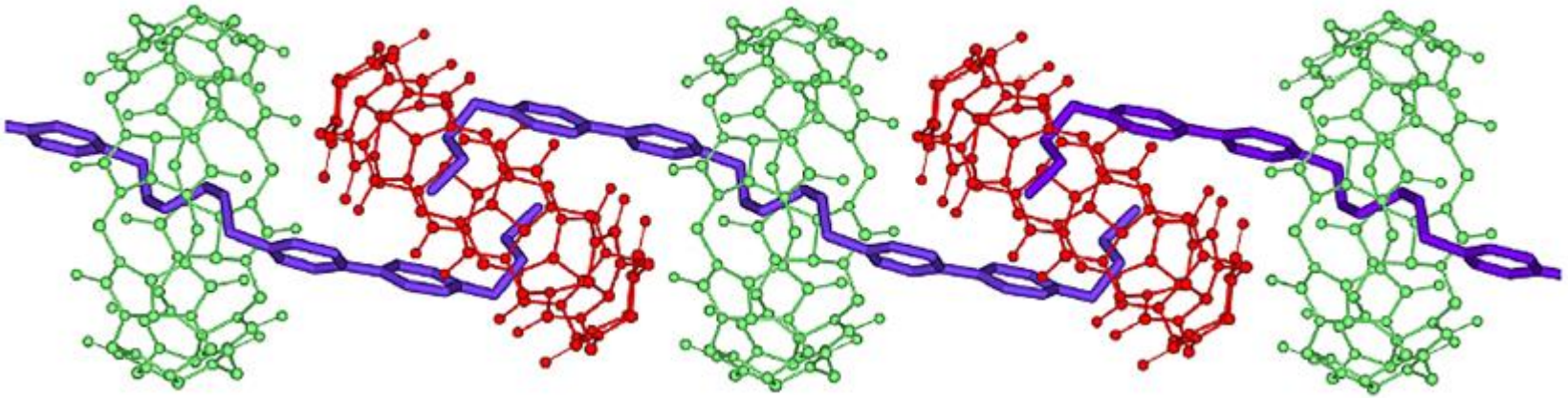
The CIF output by the latest version of SHELXL includes the *.res file and the hkl file used for refinement so it makes it easy to check exactly how the structure was refined.

If SQUEEZE has been used, the FAB file will also be included.

MUST HAVE

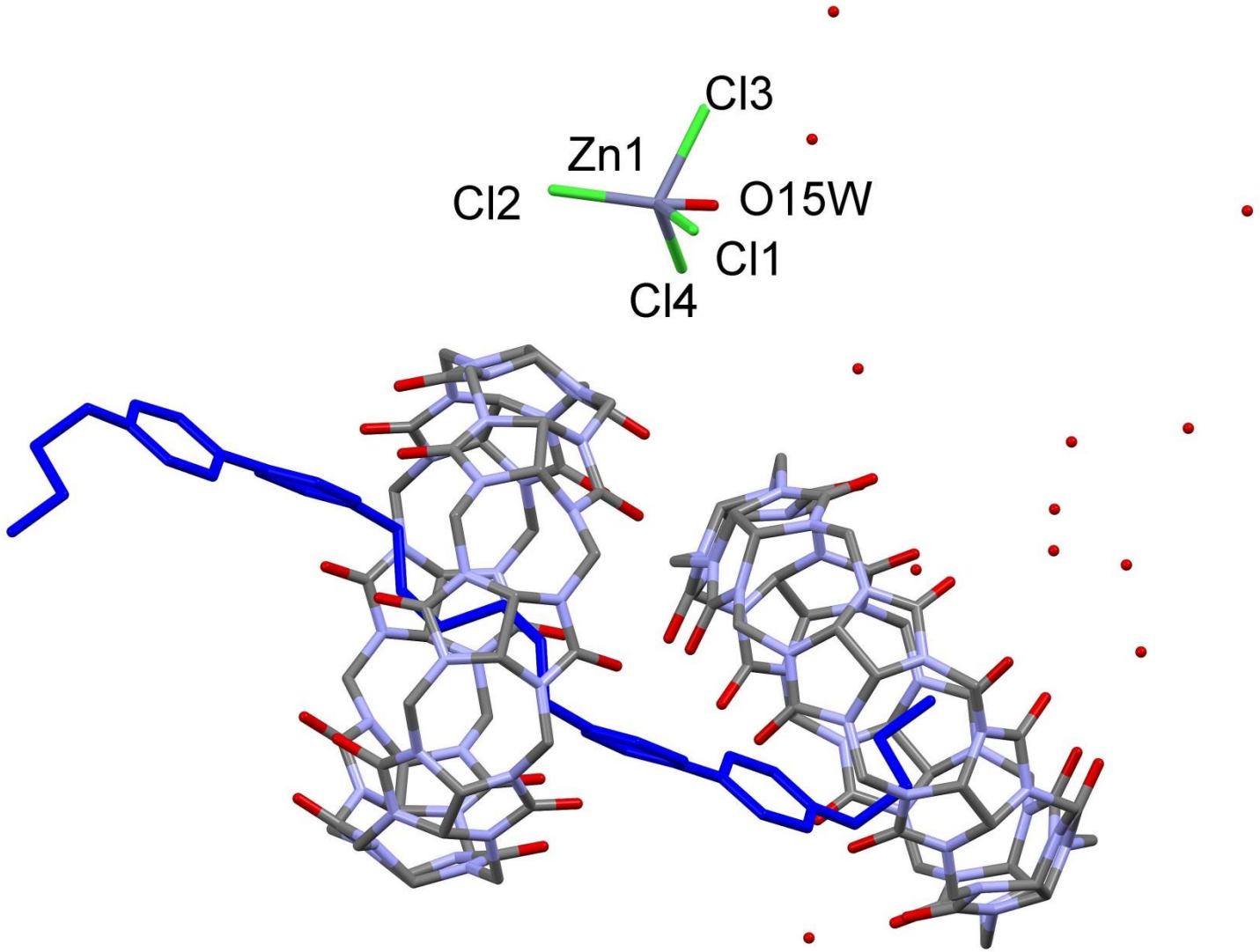






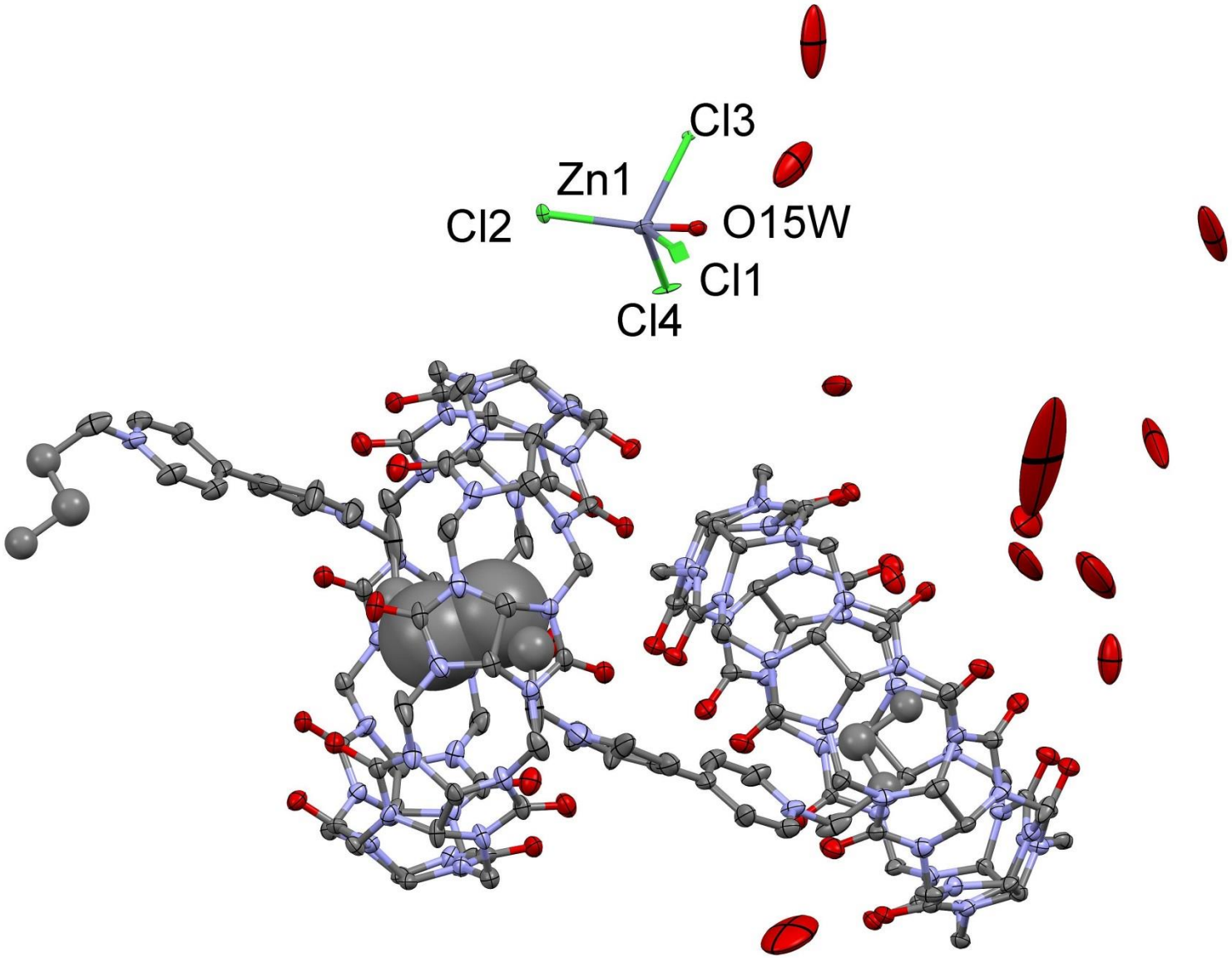
Published results

MUST HAVE

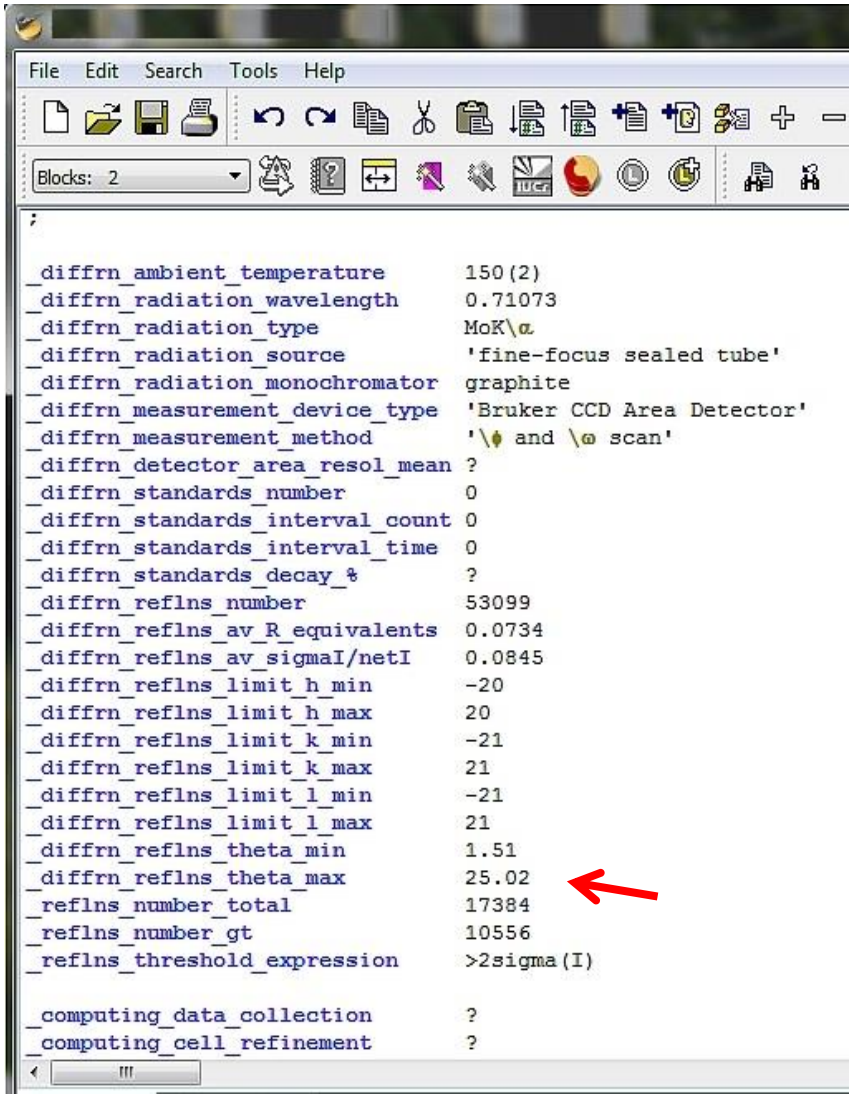


To a solution of the guest (8.30 mg, 0.010 mmol) in water (30 ml), CB8 (25.56 mg, 0.020 mmol) and $ZnCl_2$ (13.6 mg, 0.10 mmol) were added.

MUST HAVE



MUST HAVE


File Edit Search Tools Help
Blocks: 2
;
_diffrn_ambient_temperature 150(2)
_diffrn_radiation_wavelength 0.71073
_diffrn_radiation_type MoK\α
_diffrn_radiation_source 'fine-focus sealed tube'
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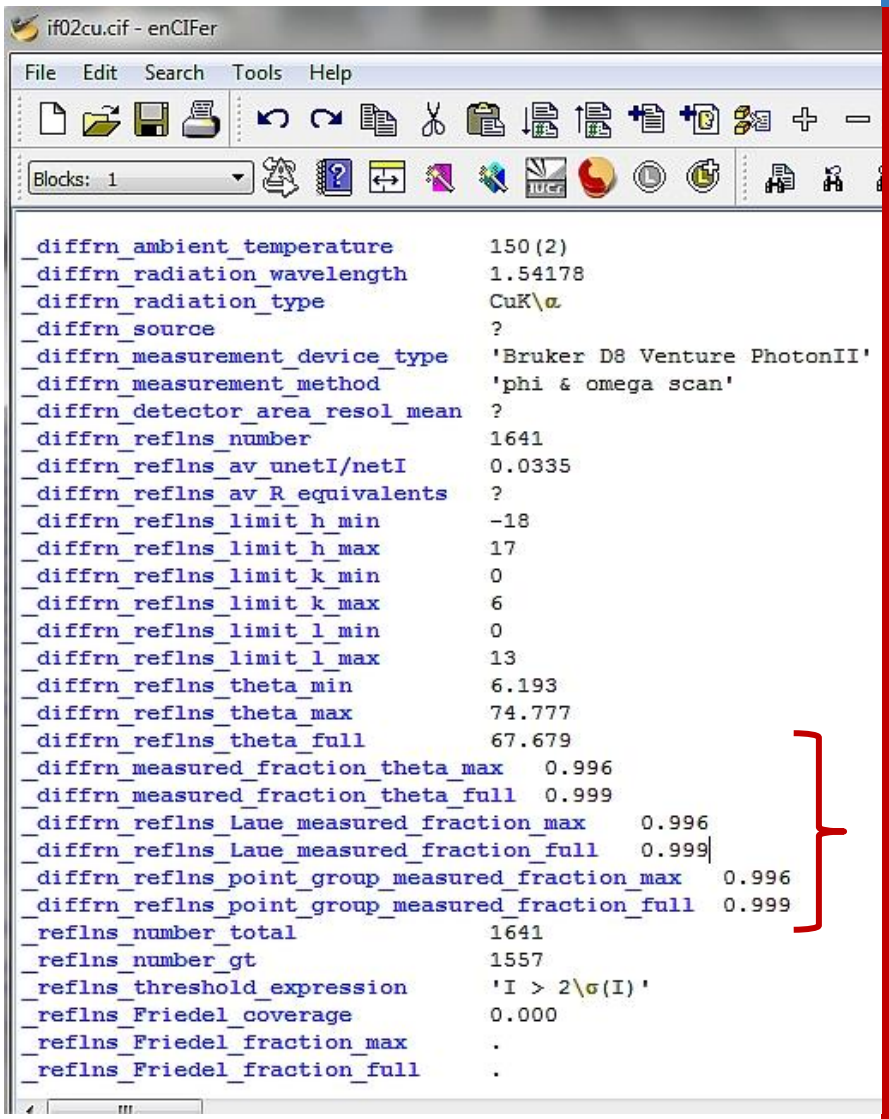
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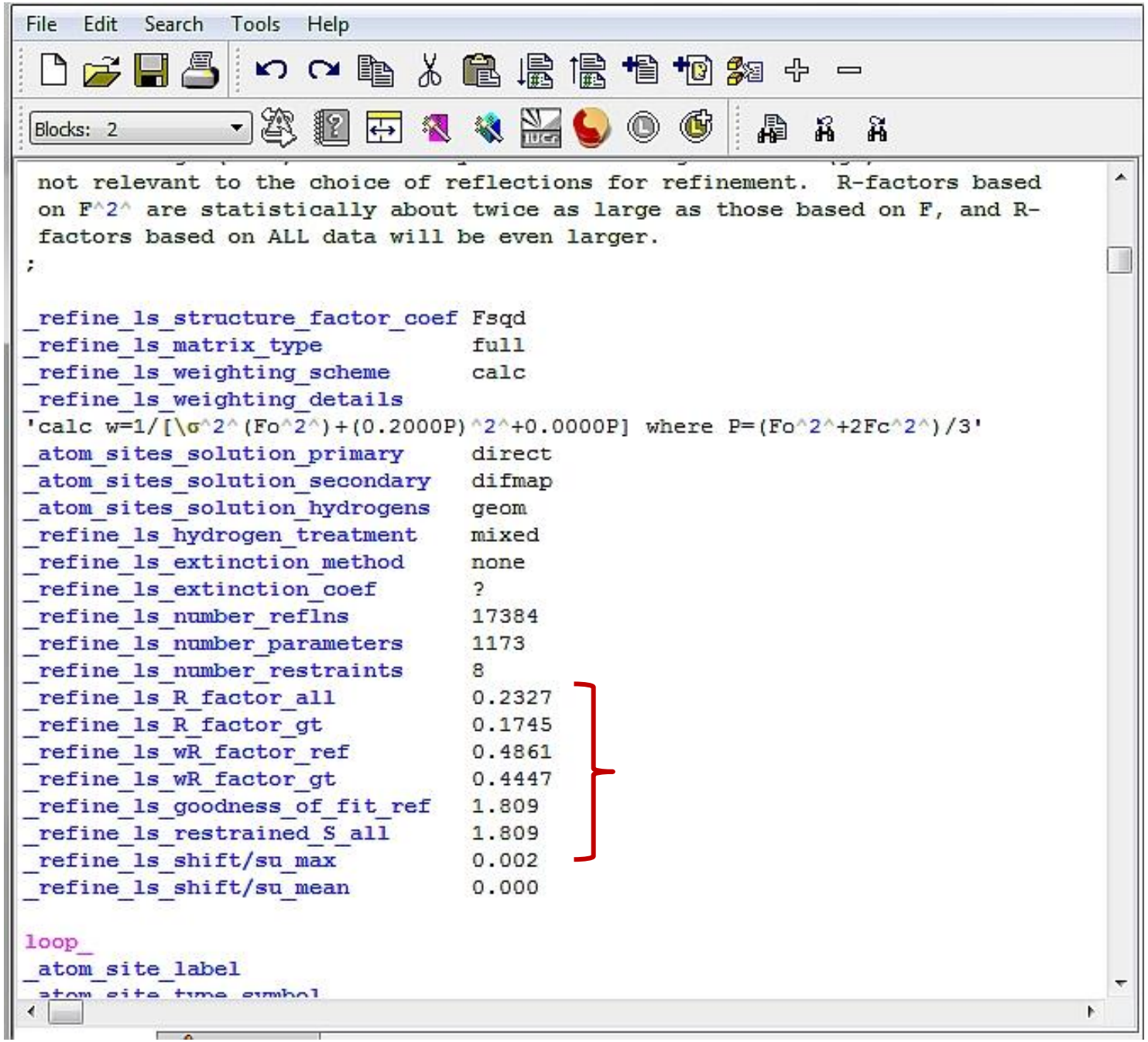
_reflns_Friedel_fraction_full .

MUST HAVE


File Edit Search Tools Help
Blocks: 2
not relevant to the choice of reflections for refinement. R-factors based
on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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_atom_sites_solution_primary direct
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loop_
_atom_site_label

MUST HAVE

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

PLAT084 ALERT 3 A	High wR2 Value (i.e. > 0.25)	0.49 Report
PLAT214 ALERT 2 A	Atom O16W (Anion/Solvent) ADP max/min Ratio	9.1 prolat
PLAT234 ALERT 4 A	Large Hirshfeld Difference C55 --C56 .	0.35 Ang.
PLAT242 ALERT 2 A	Low 'MainMol' Ueq as Compared to Neighbors of	C60 Check
PLAT260 ALERT 2 A	Large Average Ueq of Residue Including O16W	1.222 Check
PLAT430 ALERT 2 A	Short Inter D...A Contact O5W ..O14W .	2.44 Ang.
	x,y,z =	1_555 Check
PLAT430 ALERT 2 A	Short Inter D...A Contact O6W ..O14W .	2.37 Ang.
	x,y,z =	1_555 Check
PLAT602 ALERT 2 A	VERY LARGE Solvent Accessible VOID(S) in Structure	! Info

PLAT_214

ratio > 6.0	ALERT A
ratio > 5.0	ALERT B
ratio > 4.0	ALERT C

PLAT_213

ratio > 5.0	ALERT A
ratio > 4.0	ALERT B
ratio > 3.0	ALERT C

MUST HAVE

Alert level B

PLAT082_ALERT_2_B	High R1 Value	0.17 Report
PLAT097_ALERT_2_B	Large Reported Max. (Positive) Residual Density	4.45 eA-3
PLAT212_ALERT_2_B	ADP of Atom Cl1 is N.P.D. or (nearly) 2D .	Please Check
PLAT214_ALERT_2_B	Atom O8W (Anion/Solvent) ADP max/min Ratio	5.1 prolat
PLAT221_ALERT_2_B	Solv./Anion Resd 3 C Ueq(max)/Ueq(min) Range	10.0 Ratio
PLAT241_ALERT_2_B	High 'MainMol' Ueq as Compared to Neighbors of	C64 Check
PLAT260_ALERT_2_B	Large Average Ueq of Residue Including	O7W 0.417 Check
PLAT260_ALERT_2_B	Large Average Ueq of Residue Including	O8W 0.650 Check
PLAT260_ALERT_2_B	Large Average Ueq of Residue Including	O9W 0.376 Check
PLAT260_ALERT_2_B	Large Average Ueq of Residue Including	O10W 0.494 Check
PLAT260_ALERT_2_B	Large Average Ueq of Residue Including	O13W 0.482 Check
PLAT260_ALERT_2_B	Large Average Ueq of Residue Including	O14W 0.514 Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O2W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O3W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O4W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O5W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O6W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O7W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O8W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O9W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O10W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O13W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O14W Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O16W Check
PLAT341_ALERT_3_B	Low Bond Precision on C-C Bonds	0.05122 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact O3W ..O7W .	2.84 Ang.
	2-x,-y,1-z =	2_756 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact O4W ..O15W .	2.60 Ang.
	x,y,1+z =	1_556 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact O5 ..O10W .	2.78 Ang.
	x,y,z =	1_555 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact O6W ..O7 .	2.75 Ang.
	x,y,z =	1_555 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact O8W ..O8W .	2.78 Ang.
	2-x,-y,2-z =	2_757 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact O8W ..O10 .	2.80 Ang.
	x,y,z =	1_555 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact O10W ..O14W .	2.72 Ang.
	x,y,z =	1_555 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact O13W ..O16 .	2.61 Ang.
	x,y,z =	1_555 Check

https://journals.iucr.org/e/services/authorservices.html

http://journals.iucr.org/e/services/notesforauthors.html

HOW TO

Research Communications

OUTLINE

- Abstract

-Chemical context

-Structural commentary

-Supramolecular features

-Database survey

-Synthesis /crystallization

-Refinement

-An ellipsoid plot and/or a polyhedral plot for each inorganic structure.

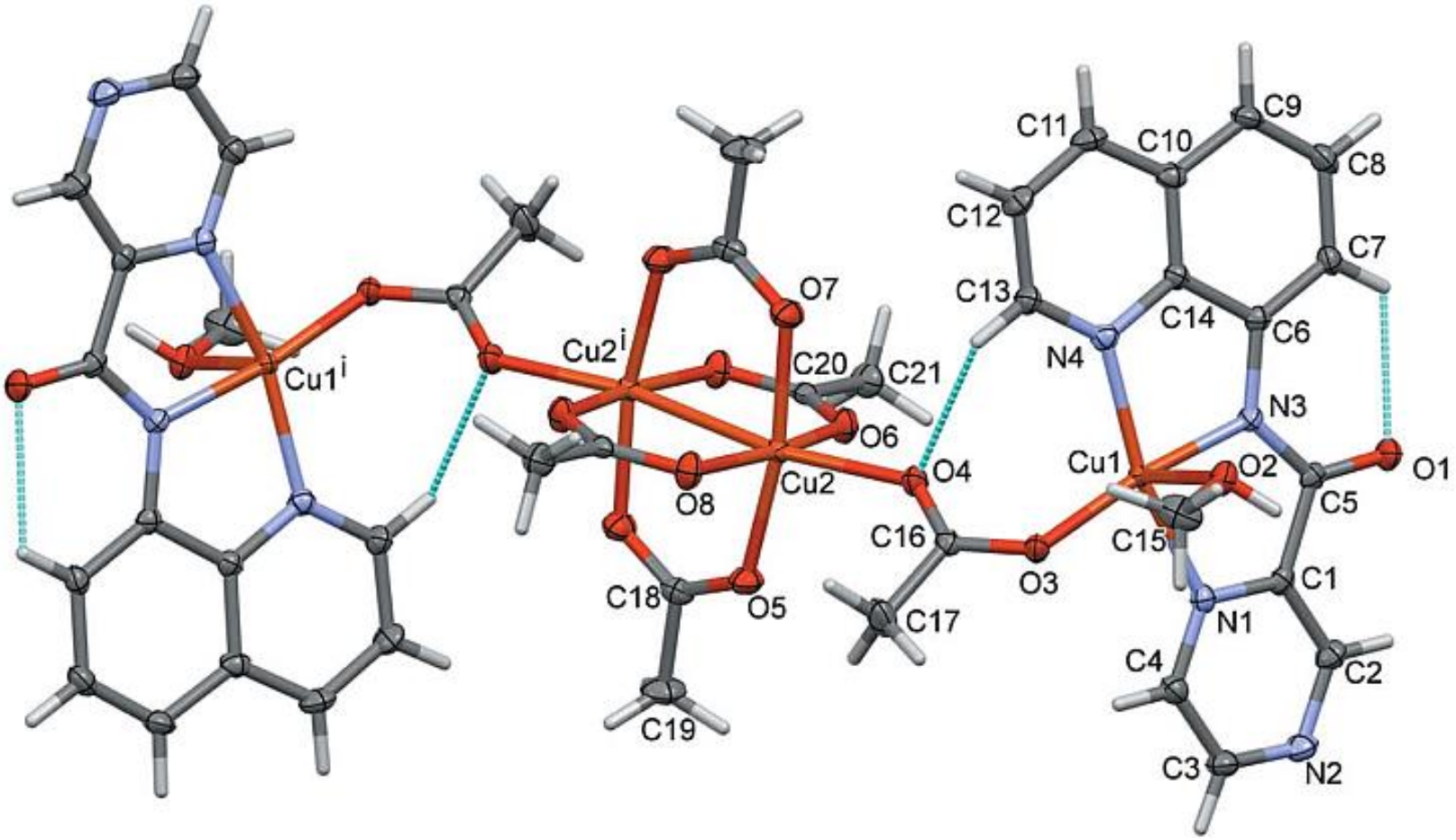
-A packing diagram

-A chemical scheme

-Tables

HOW TO

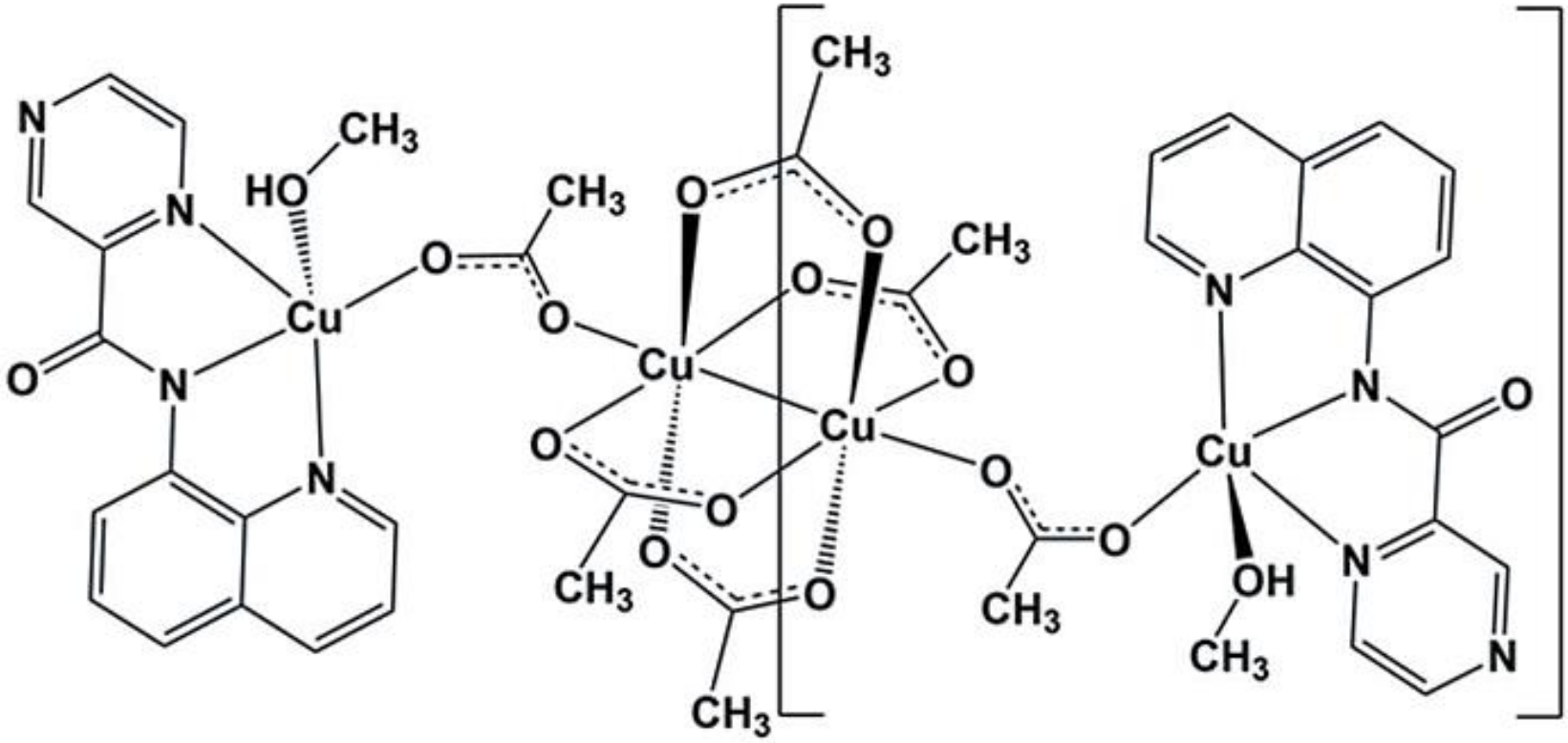
Structural commentary – ortep plot



A view of the molecular structure of complex I, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. The unlabelled atoms are related to labelled atoms by inversion symmetry [symmetry code: (i) x + 1, y, z + 1]

HOW TO

Structural commentary – chemical scheme



Acta Cryst. (2019). E**75**, 755-761

HOW TO

Structural commentary - Tables

Table 1
Selected geometric parameters (Å, °).

Fe1—N1^{i}	2.0982 (14)	Fe1—N11^{i}	2.2576 (13)
Fe1—N1	2.0982 (14)	Fe1—N31	2.2597 (13)
Fe1—N11	2.2576 (13)	Fe1—N31^{i}	2.2597 (13)
N1^{i}—Fe1—N1	180.0	N11—Fe1—N31	88.15 (5)
N1^{i}—Fe1—N11	88.79 (5)	N11^{i}—Fe1—N31	91.85 (5)
N1—Fe1—N11	91.21 (5)	N1^{i}—Fe1—N31^{i}	89.79 (5)
N1^{i}—Fe1—N11^{i}	91.21 (5)	N1—Fe1—N31^{i}	90.21 (5)
N1—Fe1—N11^{i}	88.79 (5)	N11—Fe1—N31^{i}	91.85 (5)
N11—Fe1—N11^{i}	180.0	N11^{i}—Fe1—N31^{i}	88.15 (5)
N1^{i}—Fe1—N31	90.21 (5)	N31—Fe1—N31^{i}	180.00 (7)
N1—Fe1—N31	89.79 (5)		

Symmetry code: (i) $-x, -y+1, -z+1$.

Table 1
Selected geometric parameters (Å, °).

Fe1—N1	2.0982 (14)	Fe1—N31	2.2597 (13)
Fe1—N11	2.2576 (13)		
N1^{i}—Fe1—N11	88.79 (5)	N1—Fe1—N31	89.79 (5)
N1—Fe1—N11	91.21 (5)	N11—Fe1—N31	88.15 (5)
N1^{i}—Fe1—N31	90.21 (5)	N11^{i}—Fe1—N31	91.85 (5)

Symmetry code: (i) $-x, -y+1, -z+1$.

HOW TO

Structural commentary - *Varia*

- No bond length or angle Table for structures of organic compounds; bond lenghts (and angles) for inorganic and metal-organic structures.

- Remember to use the BOND $H instructions during refinement to include the C-H bond lengths and angles in the CIF. Instruction CONF includes torsion angles.

- Standard uncertainties (s.u.) must be given for all the values reported in the discussion. They should be on the scale of the least significant digits of the result (maximum allowed value:19).

HOW TO

Synthesis/ crystallization

Crystallization conditions / solvent/ solvent ratios

Refinement – H atoms

_refine_ls_hydrogen_treatment

H atom treatment must be detailed in the experimental section

Example: The C-bound H atoms were placed in calculated positions and refined using a riding model: C—H = 0.95-0.98 A ° with Uiso(H) = 1.5Ueq(C-methyl) and 1.2Ueq(C) for other H atoms. The hydroxyl H atom was located in a difference-Fourier map and freely refined

Riding H atoms do not have s.u.

HOW TO

Supramolecular features – Tables

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the aromatic rings C9*B*–C14*B*, C9*D*–C14*D* and C1*A*–C6*A*, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1B^{i}—H1B^{i}···F1	0.95	2.41	3.344 (3)	169
C14B^{ii}—H14B^{ii}···F2	0.95	2.57	3.357 (3)	140
C7C^{ii}—H7$C3^{ii}$···F2	0.98	2.62	3.484 (2)	147
C8C^{i}—H8$C1^{i}$···F2	0.98	2.49	3.379 (3)	150
C1D^{i}—H1D^{i}···F2	0.95	2.60	3.439 (2)	147
C11A^{iii}—H11A^{iii}···F3	0.95	2.45	3.254 (2)	142
C7*D*—H7*D*1···*Cg*1^{v}	0.98	2.80	3.524 (4)	131
C7*B*—H7*B*1···*Cg*2^{vi}	0.98	2.88	3.530 (4)	124
C8*D*—H8*D*2···*Cg*3^{vii}	0.98	2.87	3.594 (3)	131

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+1, -y+1, -z$; (iii) $x, y, z-1$; (v) $x-1, y, z$; (vi) $x+1, y, z$; (vii) $-x, -y+2, -z+1$.

Angles > 120°

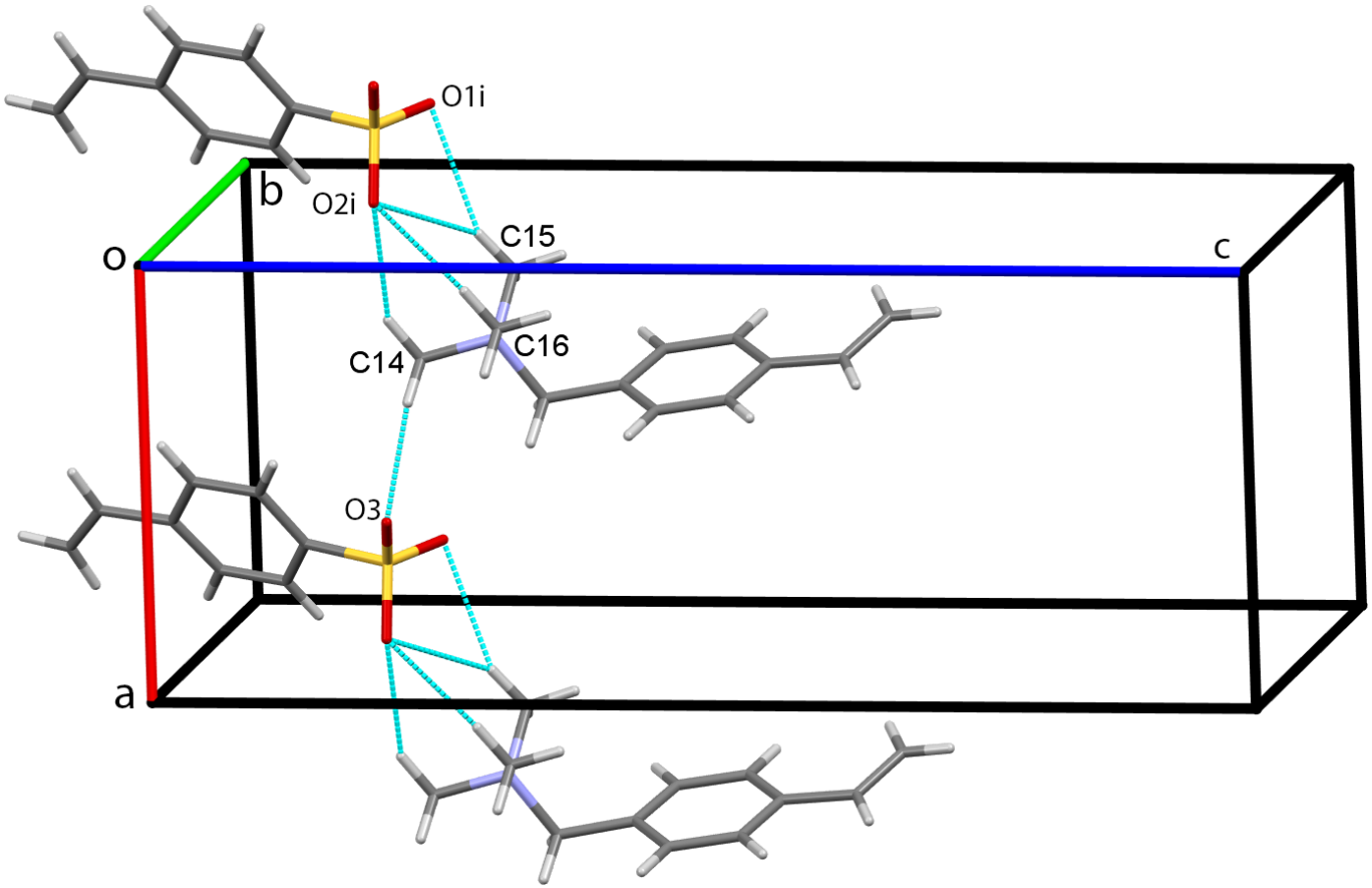
HTAB

No s.u. values for parameters which are fixed by symmetry, geometry or other constraints

Acta Cryst. (2017). E**73**, 1801-1805

H O W T O

Supramolecular features - packing diagrams



Chains of cations and anions of (I) along the *a* axis. Hydrogen bonds areshown as cyan dotted lines [symmetry code: (i) x-1,y, z].

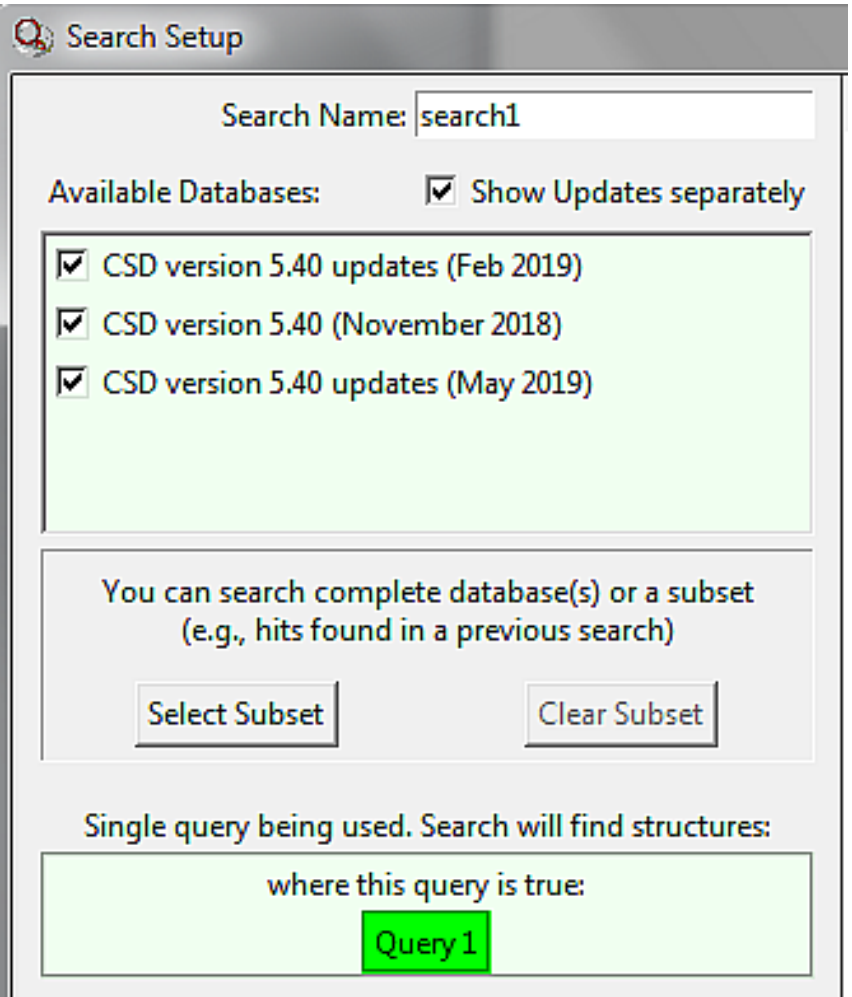
Acta Cryst. (2019). E**75**, 946-950

HOW TO

Database survey

Indicate the version of the CSD which has been used

e.g. Version 5.40, update of November 2018



Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016) *Acta Cryst. B72*, 171–179.

Cite refcodes

HOW TO

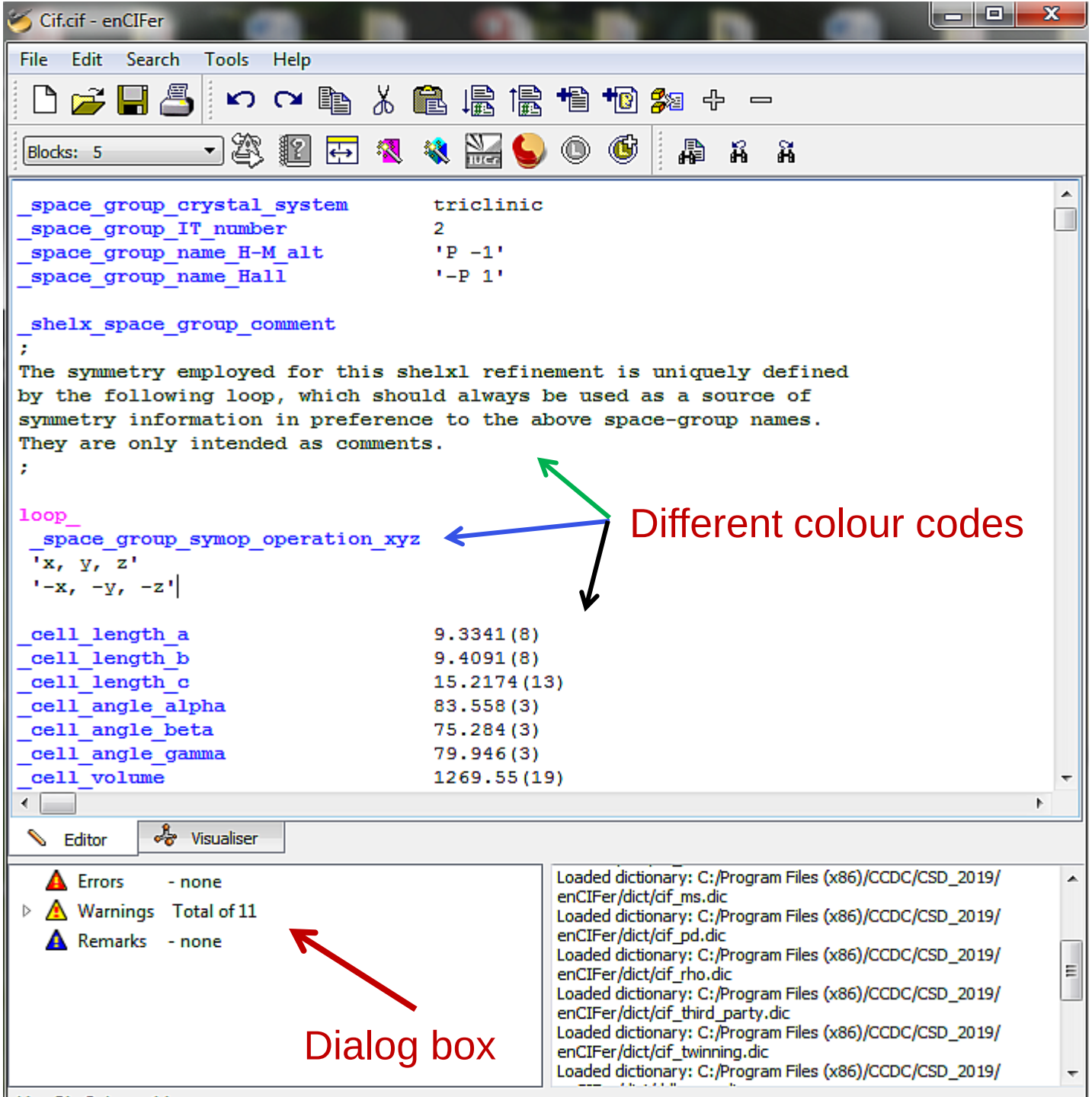
ENCIFER

graphical interface for editing CIF files (free download from the CCDC)

https://www.ccdc.cam.ac.uk/Community/csd-community/encifer/

Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004) J. Appl. Cryst. 37, 335-338.

TOOLS



Easy access to multiple structures

Different colour codes

Dialog box

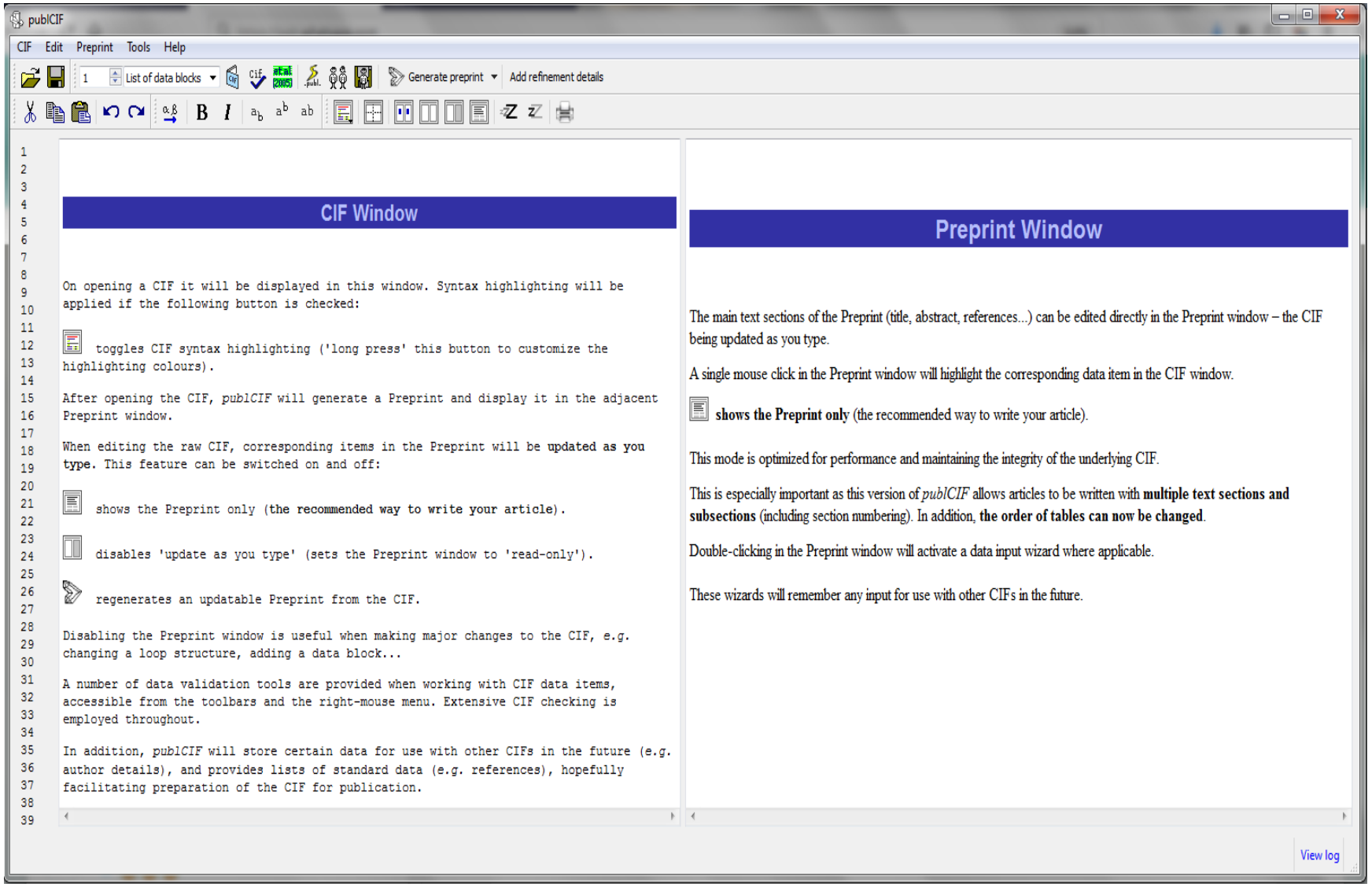
TOOLS

publCIF
free software to edit and preview a CIF for publication

http://journals.iucr.org/services/cif/publcif/

Westrip, S. P. (2010) J. Appl. Cryst. 43, 920–925

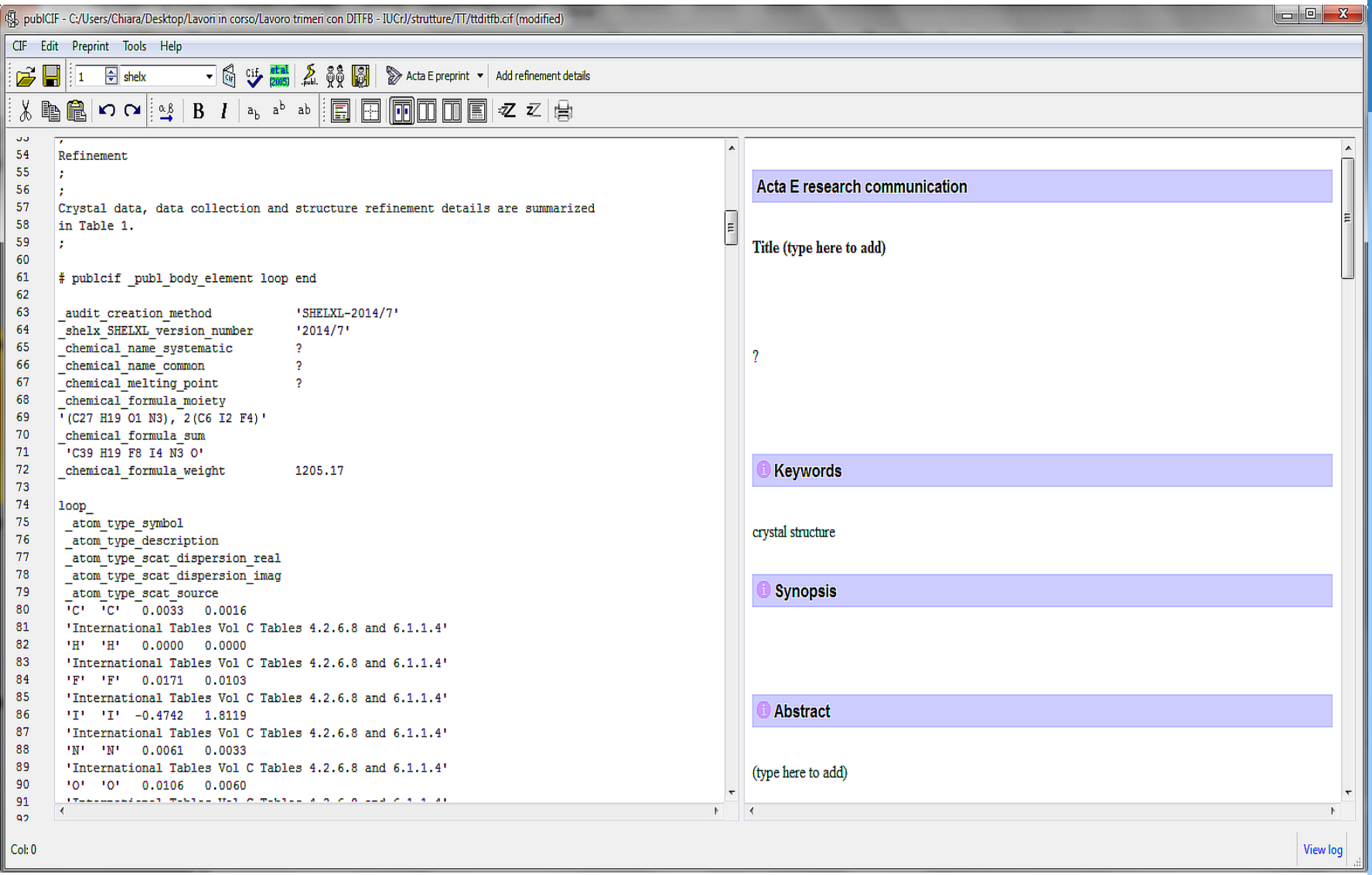
TOOLS



ASCII CIF EDITOR **WORD-TYPE EDITOR**

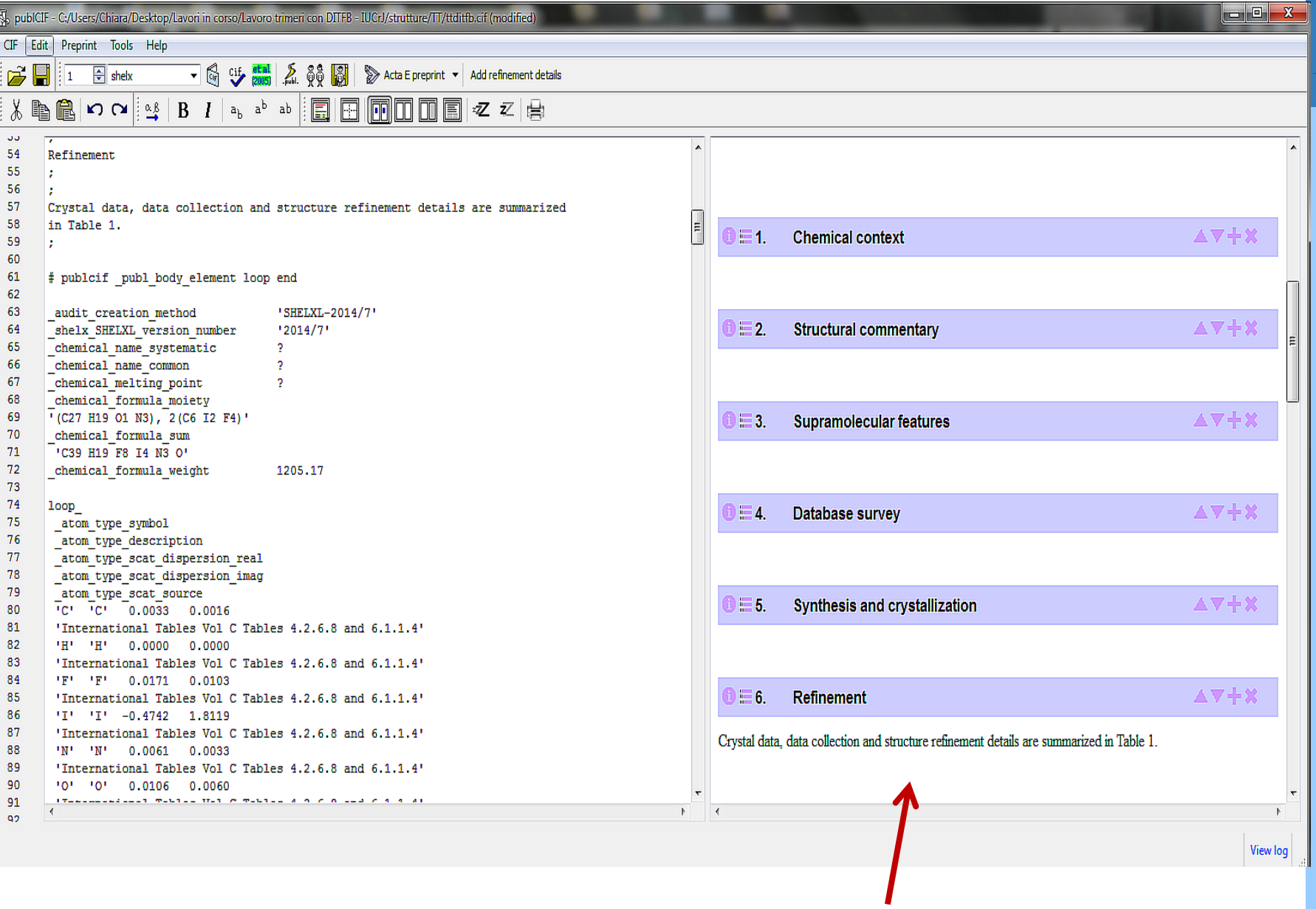
As you type in the CIF window, the Preprint window will be updated and *vice versa*.

TOOLS



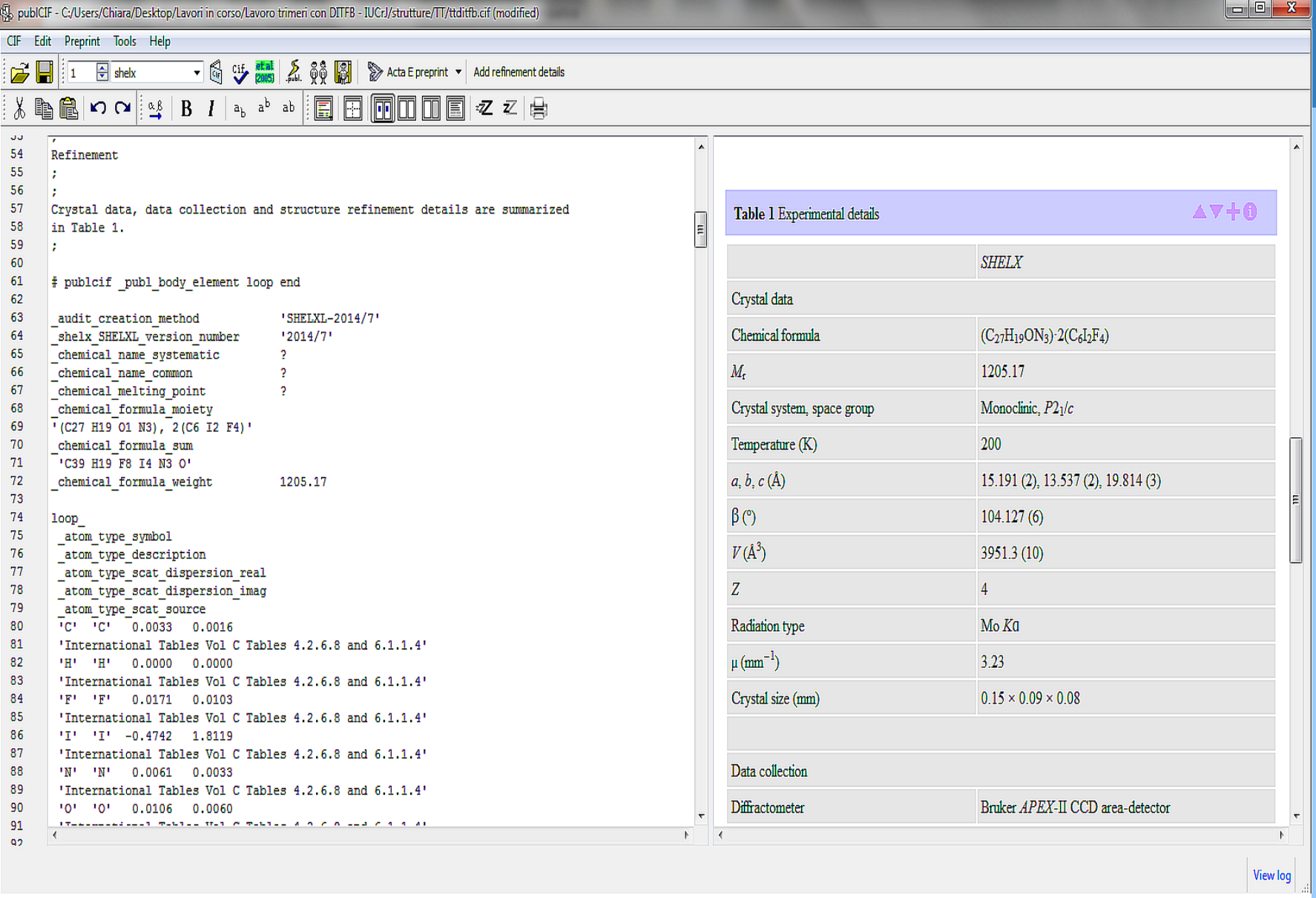
When a CIF is open, it is shown in the ascii editor. In the right part it is possible to type the paper itself.

TOOLS



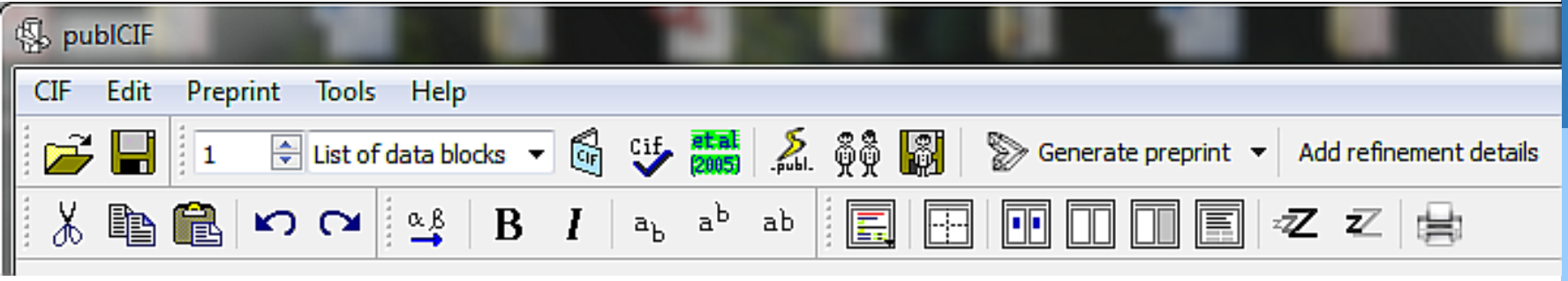
TOOLS

Standard sections of an Acta E paper

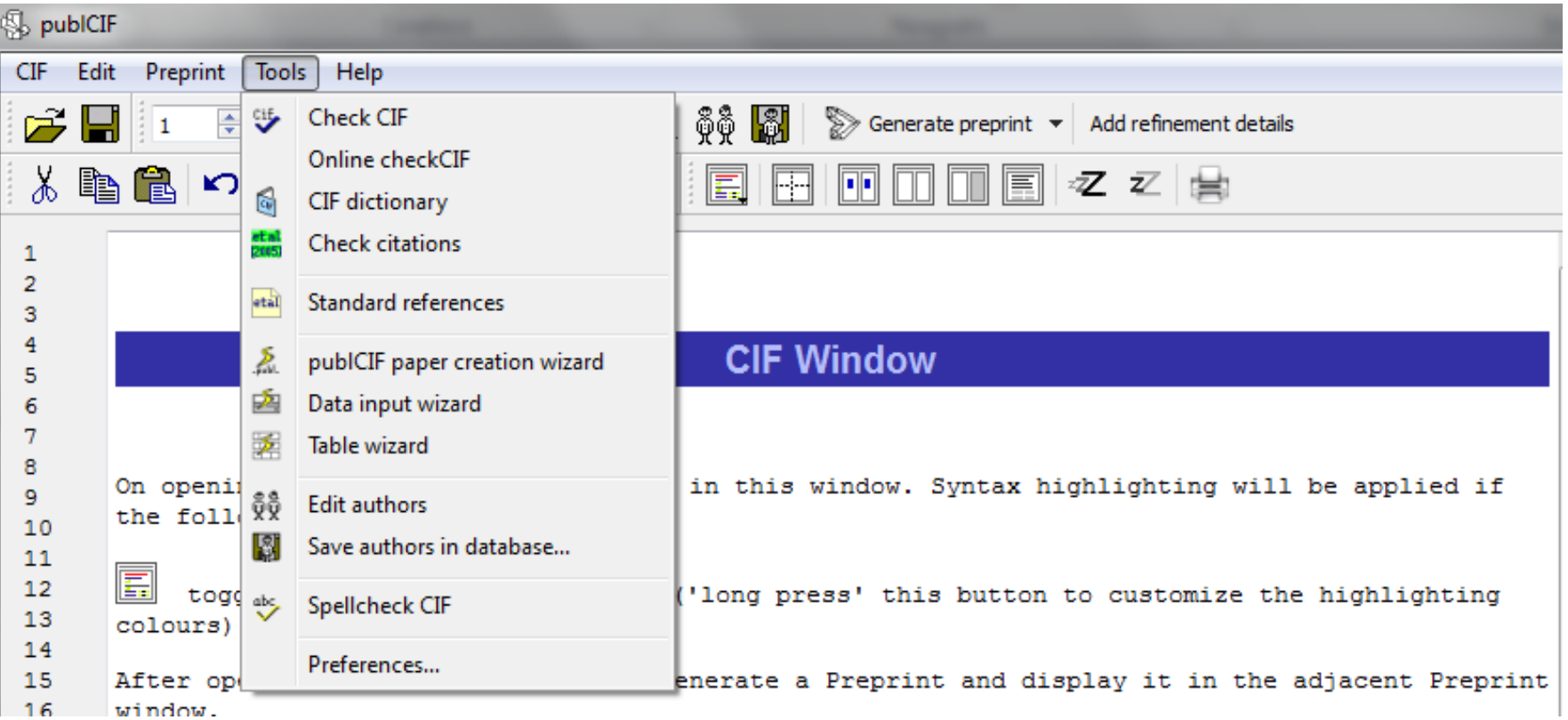


TOOLS

The experimental details are automatically formatted in a Table



Several tools to help formatting the paper



TOOLS

publCIF help

HELP DOCUMENT AVAILABLE

TOOLS

publCIF – free software to edit and preview a CIF for publication

New in this version

New publication

This release of *publCIF* introduces IUCrData – the new home for *Data Reports* previously published in Acta Cryst. E.

Data Reports in IUCrData have a fixed format tailored to a concise description of the structure, synthesis and crystallization, and any unusual aspect of the refinement process.

Getting started

If you are using *publCIF* for the first time, it is recommended that you open a trial CIF to familiarize yourself with *publCIF*'s functions