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 = 0.0036 A          Wavelength=1.54184

Cell:          a=8.4016(4)        b=15.5626(5)      c=16.3803(7)
               alpha=101.944(3)   beta=104.296(4)   gamma=102.394(3)
Temperature:   150 K
```

	Calculated	Reported
Volume	1949.09(15)	1949.09(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C40 H44 Cu2 N8 O6	C40 H44 Cu2 N8 O6
Sum formula	C40 H44 Cu2 N8 O6	C40 H44 Cu2 N8 O6
Mr	859.93	859.93
Dx,g cm-3	1.465	1.465
Z	2	2
Mu (mm-1)	1.824	1.824
F000	892.0	892.0
F000'	886.47	
h,k,lmax	10,19,20	10,19,20
Nref	7670	7466
Tmin,Tmax	0.850,0.977	0.960,0.980
Tmin'	0.696	

```
Correction method= # Reported T Limits: Tmin=0.960 Tmax=0.980
AbsCorr = MULTI-SCAN

Data completeness= 0.973          Theta(max)= 72.084

R(reflections)= 0.0350( 6388)     wR2(reflections)= 0.0894( 7466)

S = 0.987                 Npar= 530
```

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 C

```
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range        4.6 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C39    --  C40     ..       0.16 Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600         33 Report
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          6 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          4 Report
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF     Please Do !
PLAT300_ALERT_4_G Atom Site Occupancy of >H391   is Constrained at      0.572 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H392   is Constrained at      0.572 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H401   is Constrained at      0.572 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H402   is Constrained at      0.572 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >H403   is Constrained at      0.572 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H1391  is Constrained at      0.428 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H1392  is Constrained at      0.428 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H1401  is Constrained at      0.428 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H1402  is Constrained at      0.428 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H1403  is Constrained at      0.428 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1)..          4 % Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          5 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         25 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)           2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        170 Note
PLAT960_ALERT_3_G Number of Intensities with I  <   - 2*sig(I) ...          7 Check
```

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
19 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
13 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Publication of your CIF

You should attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. *checkCIF* was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 24/11/2016; check.def file version of 23/11/2016

Datablock I - ellipsoid plot