checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 15501_yn-56

```
Bond precision:  C-C = 0.0033 A          Wavelength=1.54184

Cell:            a=11.5109(1)    b=21.0713(2)       c=20.3473(3)
                 alpha=90        beta=98.719(1)     gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	4878.20(10)	4878.20(10)
Space group	I 2/a	I 1 2/a 1
Hall group	-I 2ya	-I 2ya
Moiety formula	C36 H32 Cu2 N4 O14 S4, 2(C4 H8 O)	C18 H16 Cu N2 O7 S2, C4 H8 O
Sum formula	C44 H48 Cu2 N4 O16 S4	C22 H24 Cu N2 O8 S2
Mr	1144.20	572.09
Dx,g cm-3	1.558	1.558
Z	4	8
Mu (mm-1)	3.310	3.310
F000	2360.0	2360.0
F000’	2356.12	
h,k,lmax	14,25,24	14,25,24
Nref	4625	4625
Tmin,Tmax	0.767,0.876	0.817,1.000
Tmin’	0.767	

```
Correction method= # Reported T Limits: Tmin=0.817 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 69.994

R(reflections)= 0.0296( 4385)     wR2(reflections)= 0.0861( 4625)

S = 1.060                 Npar= 318
```

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 NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.2 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O2       --C1       .        5.5 s.u.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C15 Check
```

Alert level G

```
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       7.27 Why ?
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing ..............    0.00020 Ang.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1      --O2       .        5.3 s.u.
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O1S            108.4 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          8 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.19 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2       (II)      .       2.20 Info
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          1 Note
```

```
   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
  10 ALERT level G = General information/check it is not something unexpected

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

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT220_15501_yn-56
;
PROBLEM: NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.2 Ratio
RESPONSE: ...
;
_vrf_PLAT230_15501_yn-56
;
PROBLEM: Hirshfeld Test Diff for    O2       --C1       .        5.5 s.u.
RESPONSE: ...
;
_vrf_PLAT242_15501_yn-56
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of        C15 Check
RESPONSE: ...
;
# end Validation Reply Form
```

It is advisable to 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 purpose of your study may justify the reported deviations and the more serious of these should normally 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.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/03/2021; check.def file version of 19/03/2021

Datablock 15501_yn-56 - ellipsoid plot