

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: 1b

Bond precision: C-C = 0.0200 A Wavelength=0.71069

Cell: a=7.3890(19) b=8.473(2) c=9.491(2)
 alpha=70.273(5) beta=67.170(5) gamma=84.949(5)

Temperature: 296 K

	Calculated	Reported
Volume	514.9(2)	514.9(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C6 H8 Br Cu N2 S3	C6 H8 Br Cu N2 S3
Sum formula	C6 H8 Br Cu N2 S3	C6 H8 Br Cu N2 S3
Mr	347.80	347.80
Dx,g cm-3	2.243	2.243
Z	2	2
Mu (mm-1)	6.560	6.560
F000	340.0	340.0
F000'	340.90	
h,k,lmax	8,10,11	8,10,11
Nref	1951	1888
Tmin,Tmax	0.497,0.675	0.483,0.745
Tmin'	0.451	

Correction method= MULTI-SCAN

Data completeness= 0.968 Theta(max)= 25.660

R(reflections)= 0.0679(1742) wR2(reflections)= 0.2204(1888)

S = 1.247 Npar= Npar = 118

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 B

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.0200 Ang.

🟢 Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.967 Note
PLAT213_ALERT_2_C Atom C5 has ADP max/min Ratio 3.2 prolat

🟠 Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 32.87 Why ?
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal 0.00500 Degree
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) 1.69 Note

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
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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*, 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 05/02/2014; check.def file version of 05/02/2014

Datablock 1b - ellipsoid plot

