

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_062517

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: cu_062517

Bond precision: C-C = 0.0088 A

Wavelength=1.54178

Cell: a=7.3341(5) b=7.6637(5) c=12.6658(9)
 alpha=94.557(2) beta=98.228(2) gamma=114.796(2)
Temperature: 100 K

	Calculated	Reported
Volume	631.86(8)	631.86(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C9 H18 Cl Ga N2 S2	C9 H18 Cl Ga N2 S2
Sum formula	C9 H18 Cl Ga N2 S2	C9 H18 Cl Ga N2 S2
Mr	323.54	323.54
Dx,g cm-3	1.701	1.701
Z	2	2
Mu (mm-1)	7.767	7.767
F000	332.0	332.0
F000'	331.90	
h,k,lmax	8,8,14	8,8,14
Nref	1962	1862
Tmin,Tmax	0.911,0.925	0.049,0.156
Tmin'	0.460	

Correction method= # Reported T Limits: Tmin=0.049 Tmax=0.156
AbsCorr = MULTI-SCAN

Data completeness= 0.949

Theta(max)= 61.257

R(reflections)= 0.0498(1851)

wR2(reflections)= 0.1392(1862)

S = 1.040

Npar= 136

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

THETM01_ALERT_3_B The value of $\sin(\theta_{\max})/\lambda$ is less than 0.575
Calculated $\sin(\theta_{\max})/\lambda = 0.5687$

Author Response: Data was collected on a Bruker Venture instrument with Cu-source.

PLAT029_ALERT_3_B _diffn_measured_fraction_theta_full value Low . 0.949 Note

Author Response: Data was collected on a Bruker Venture instrument with Cu-source. Triclinic spacegroup.



Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density	2.79	Report
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds	0.0088	Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.569	100	Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.	0	Note



Alert level G

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)	0.002	Degree
PLAT793_ALERT_4_G The Model has Chirality at N1 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G The Model has Chirality at N2 (Centro SPGR)	R	Verify
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) Still	98 %	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
4 **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
5 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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.

