

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

Bond precision: C-C = 0.0022 A Wavelength=1.54178

Cell: a=11.90994(6) b=13.21619(7) c=26.83905(13)
 alpha=90 beta=97.6274(4) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	4187.20(4)	4187.20(4)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C23 H22 B Cu N P S	C23 H22 B Cu N P S
Sum formula	C23 H22 B Cu N P S	C23 H22 B Cu N P S
Mr	449.81	449.79
Dx,g cm-3	1.427	1.427
Z	8	8
Mu (mm-1)	3.175	3.175
F000	1856.0	1856.0
F000'	1848.69	
h,k,lmax	14,16,32	14,15,32
Nref	3983	3963
Tmin,Tmax	0.757,0.798	0.745,0.975
Tmin'	0.628	

Correction method= # Reported T Limits: Tmin=0.745 Tmax=0.975
AbsCorr = GAUSSIAN

Data completeness= 0.995 Theta(max)= 70.065

R(reflections)= 0.0244(3908) wR2(reflections)= 0.0664(3963)

S = 1.072 Npar= 290

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**

PLAT420_ALERT_2_C	D-H Without Acceptor	Cu1	--H1AA	.	Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor	Cu1	--H1AB	.	Please Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=		0.600		2 Report

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite				16 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...				8 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large				5.52 Why ?
PLAT142_ALERT_4_G	s.u. on b - Axis Small or Missing				0.00007 Ang.
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing				0.00013 Ang.
PLAT145_ALERT_4_G	s.u. on beta Small or Missing				0.0004 Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records				2 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records				1 Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records				13 Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records				1 Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for S1A --C1A				8.7 s.u.
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)				14% Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels				6 Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				68 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=		0.600		15 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...				2 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				16 Info

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
17 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
9 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.

PLATON version of 03/05/2019; check.def file version of 29/04/2019

