

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cd052-1_twin1_hklf5

No syntax errors found. CIF dictionary Interpreting this report

Datablock: cd052-1_twin1_hklf5

Bond precision: C-C = 0.0093 A Wavelength=0.71073
Cell: a=12.713(4) b=10.108(4) c=10.835(5)
alpha=90 beta=91.21(3) gamma=90
Temperature: 110 K

	Calculated	Reported
Volume	1392.0(10)	1392.0(9)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C10 H8 Br2 N2 S2 Zn	C10 H8 Br2 N2 S2 Zn
Sum formula	C10 H8 Br2 N2 S2 Zn	C10 H8 Br2 N2 S2 Zn
Mr	445.51	445.49
Dx,g cm ⁻³	2.126	2.126
Z	4	4
Mu (mm ⁻¹)	7.783	7.782
F000	856.0	856.0
F000'	856.21	
h,k,lmax	17,13,14	16,13,14
Nref	1838	2861
Tmin,Tmax	0.525,0.678	0.388,0.697
Tmin'	0.308	

Correction method= MULTI-SCAN

Data completeness= 1.557 Theta(max)= 28.920

R(reflections)= 0.0531(1659) wR2(reflections)= 0.1190(2861)

S = 0.901 Npar= 79

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

PLAT021_ALERT_1_B Ratio Unique / Expected Reflections too High ... 1.557

Alert level C

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds	0.0093 Ang
PLAT906_ALERT_3_C Large K value in the Analysis of Variance	6.142
PLAT906_ALERT_3_C Large K value in the Analysis of Variance	2.061
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min)	1

● **Alert level G**

PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .	1
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..	!
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	125
PLAT931_ALERT_5_G Check Twin Law () [0 0 1] Estimated BASF	0.29

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **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
 0 ALERT type 2 Indicator that the structure model may be wrong or deficient
 4 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

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 05/11/2012; check.def file version of 05/11/2012

