

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: q17_a37sadm-2_pl

Bond precision:	C-C = 0.0089 A	Wavelength=0.71073
Cell:	a=9.2972(19)	b=14.257(3) c=13.200(3)
	alpha=90	beta=101.844(3) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	1712.4(6)	1712.4(6)
Space group	P 21	P2(1)
Hall group	P 2yb	?
Moiety formula	C13 H26 Br2 N4 Zn	C13 H26 Br2 N4 Zn
Sum formula	C13 H26 Br2 N4 Zn	C13 H26 Br2 N4 Zn
Mr	463.57	463.57
Dx,g cm-3	1.798	1.798
Z	4	4
Mu (mm-1)	6.098	6.098
F000	928.0	928.0
F000'	927.19	
h,k,lmax	11,17,16	11,17,16
Nref	7167[3733]	7045
Tmin,Tmax	0.256,0.314	0.335,0.390
Tmin'	0.237	

Correction method= # Reported T Limits: Tmin=0.335 Tmax=0.390
AbsCorr = MULTI-SCAN

Data completeness= 1.89/0.98 Theta(max)= 26.560

R(reflections)= 0.0455(6311) wR2(reflections)= 0.1164(7045)

S = 1.027 Npar= 385

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

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00889 Ang.
 PLAT420_ALERT_2_C D-H Without Acceptor N24 -- H103 ... Please Check



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 5 Note
 PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 1 Report
 PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
 PLAT111_ALERT_2_G ADDSYM Detects New (Pseudo) Centre of Symmetry . 85 %Fit
 PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space Group P21/n Check
 PLAT791_ALERT_4_G The Model has Chirality at C6 (Chiral SPGR) S Verify
 PLAT791_ALERT_4_G The Model has Chirality at C9 (Chiral SPGR) R Verify
 PLAT791_ALERT_4_G The Model has Chirality at C26 (Chiral SPGR) S Verify
 PLAT791_ALERT_4_G The Model has Chirality at C28 (Chiral SPGR) R Verify
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 10 Note
 PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2016 Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 11 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 5 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
 5 ALERT type 4 Improvement, methodology, query or suggestion
 1 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.

Datablock q17_a37sadm-2_pl - ellipsoid plot

