

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3075

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: 3075

Bond precision: C-C = 0.0050 Å

Wavelength=0.71073

Cell: a=10.9344(4) b=14.4572(5) c=15.7160(6)
 alpha=65.850(4) beta=75.359(3) gamma=87.591(3)
Temperature: 173 K

	Calculated	Reported
Volume	2188.04(16)	2188.05(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C38 H44 Br2 Fe2 N2 O3 Si2 Zn, C3 H6 O1.02	C38 H44 Br2 Fe2 N2 O3 Si2 Zn, C3 H6 O1.02
Sum formula	C41 H50 Br2 Fe2 N2 O4.02 Si2 Zn	C41 H50 Br2 Fe2 N2 O4.02 Si2 Zn
Mr	1028.24	1028.22
Dx, g cm ⁻³	1.561	1.561
Z	2	2
Mu (mm ⁻¹)	3.120	3.120
F000	1044.3	1044.0
F000'	1045.77	
h,k,lmax	13,18,20	13,18,20
Nref	9544	9491
Tmin,Tmax	0.799,0.856	0.927,1.000
Tmin'	0.779	

Correction method= # Reported T Limits: Tmin=0.927 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.994

Theta(max)= 26.997

R(reflections)= 0.0358(7323)

wR2(reflections)= 0.0753(9491)

S = 1.022

Npar= 502

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 A

PLAT075_ALERT_1_A Occupancy 1.021 greater than 1.0 for 04



Alert level C

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C40 Check
 PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 45 Ang3
 PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min) 5 Note
 PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 3 Report



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note
 PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
 PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
 PLAT304_ALERT_4_G Non-Integer Number of Atoms (10.02) in Resd. # 2 Check
 PLAT396_ALERT_2_G Deviating Si-O-Si Angle from 150 Deg for O2 128.4 Degree
 PLAT793_ALERT_4_G The Model has Chirality at Si1 (Centro SPGR) R Verify
 PLAT793_ALERT_4_G The Model has Chirality at Si2 (Centro SPGR) R Verify
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 2 Note
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 46 Note
 PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 4 Note
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Note

- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
- 0 **ALERT level B** = A potentially serious problem, consider carefully
- 4 **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
- 2 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
- 3 ALERT type 3 Indicator that the structure quality may be low
- 6 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.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT075_3075
;
PROBLEM: Occupancy      1.021 greater than 1.0 for .....      04
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 24/11/2016; check.def file version of 23/11/2016

