

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3120_twin1_hklf4

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: 3120_twin1_hklf4

Bond precision:	C-C = 0.0169 Å	Wavelength=0.71073
Cell:	a=8.1910(6)	b=30.593(2) c=9.8539(7)
	alpha=90	beta=103.762(7) gamma=90
Temperature:	173 K	
	Calculated	Reported
Volume	2398.4(3)	2398.3(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C48 H56 Br2 Fe4 N2 O4 Si2 Zn2	C48 H56 Br2 Fe4 N2 O4 Si2 Zn2
Sum formula	C48 H56 Br2 Fe4 N2 O4 Si2 Zn2	C48 H56 Br2 Fe4 N2 O4 Si2 Zn2
Mr	1295.11	1295.08
Dx, g cm ⁻³	1.793	1.793
Z	2	2
Mu (mm ⁻¹)	3.924	3.924
F000	1304.0	1304.0
F000'	1307.42	
h,k,lmax	10,37,12	10,37,12
Nref	4704	9157
Tmin,Tmax	0.631,0.822	0.377,1.000
Tmin'	0.305	

Correction method= # Reported T Limits: Tmin=0.377 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.947 Theta(max)= 26.000

R(reflections)= 0.0818(5008) wR2(reflections)= 0.2662(9157)

S = 1.122 Npar= 293

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

PLAT213_ALERT_2_A Atom C8 has ADP max/min Ratio 6.6 oblate



Alert level B

PLAT230_ALERT_2_B Hirshfeld Test Diff for C6 -- C10 .. 7.1 s.u.
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.01686 Ang.



Alert level C

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.27 Report
PLAT213_ALERT_2_C Atom C9 has ADP max/min Ratio 3.2 prolat
PLAT234_ALERT_4_C Large Hirshfeld Difference Fe1 -- C8 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Fe2 -- C18 .. 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Fe2 -- C21 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N1 -- C12 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N1 -- C13 .. 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C1 -- C2 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C7 -- C8 .. 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C15 -- C16 .. 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C21 -- C22 .. 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C22 -- C23 .. 0.20 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C17 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N1 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 5.147 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 2.406 Check
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 15 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 86.65 Check



Alert level G

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.14 Report
PLAT395_ALERT_2_G Deviating X-O-Y Angle from 120 Deg for O2 126.9 Degre
PLAT793_ALERT_4_G The Model has Chirality at Si1 (Centro SPGR) S Verify
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min) 1 Note
PLAT931_ALERT_5_G Found Twin Law (1 0 -1)[] Estimated BASF 0.28 Check

- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
18 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
12 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.

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_PLAT213_3120_twin1_hklf4
;
PROBLEM: Atom C8                has ADP max/min Ratio ..... 6.6 oblate
RESPONSE: ...
;
# end Validation Reply Form
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PLATON version of 24/11/2016; check.def file version of 23/11/2016

