checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_b0662_0m

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: mo_b0662_0m

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Bond precision:  C-C = 0.0065 A          Wavelength=0.71073

Cell:            a=9.8916(13)    b=14.438(2)         c=20.415(3)
                 alpha=90        beta=102.936(5)     gamma=90
Temperature:     100 K
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	Calculated	Reported
Volume	2841.6(7)	2841.6(7)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C26 H34 Br2 Fe2 N2 O2 Si Zn	C26 H34 Br2 Fe2 N2 O2 Si Zn
Sum formula	C26 H34 Br2 Fe2 N2 O2 Si Zn	C26 H34 Br2 Fe2 N2 O2 Si Zn
Mr	771.53	771.53
Dx,g cm-3	1.804	1.803
Z	4	4
Mu (mm-1)	4.726	4.726
F000	1544.0	1544.0
F000’	1546.40	
h,k,lmax	13,20,28	13,20,28
Nref	16112[8356]	16000
Tmin,Tmax	0.385,0.597	0.006,0.024
Tmin’	0.343	

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Correction method= # Reported T Limits: Tmin=0.006 Tmax=0.024
AbsCorr = MULTI-SCAN

Data completeness= 1.91/0.99      Theta(max)= 29.671

R(reflections)= 0.0294( 14993)    wR2(reflections)= 0.0741( 16000)

S = 1.045                 Npar= 667
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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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	3.16	Report
PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem. B	86	%Fit
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C21	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Fe2	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00645	Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #	1	Note
	C26 H34 Br2 Fe2 N2 O2 Si Zn		
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0	Note

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Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2	Note
	C26 H34 Br2 Fe2 N2 O2 Si Zn		
PLAT791_ALERT_4_G	The Model has Chirality at Si1 (Chiral SPGR)	S	Verify
PLAT791_ALERT_4_G	The Model has Chirality at Si2 (Chiral SPGR)	S	Verify
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min)	3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	43	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	2	Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **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
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.

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

Datablock mo_b0662_0m - ellipsoid plot