

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3118

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: 3118

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Bond precision:	C-C = 0.0069 Å	Wavelength=0.71073
Cell:	a=15.0001(6)	b=11.2793(5)      c=27.6027(12)
	alpha=90	beta=90      gamma=90
Temperature:	173 K	
	Calculated	Reported
Volume	4670.1(3)	4670.1(3)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C46 H52 Cl2 Fe4 N2 O4 Si2 Zn2	C46 H52 Cl2 Fe4 N2 O4 Si2 Zn2
Sum formula	C46 H52 Cl2 Fe4 N2 O4 Si2 Zn2	C46 H52 Cl2 Fe4 N2 O4 Si2 Zn2
Mr	1178.16	1178.11
Dx, g cm <sup>-3</sup>	1.676	1.676
Z	4	4
Mu (mm <sup>-1</sup> )	2.431	2.431
F000	2400.0	2400.0
F000'	2410.14	
h,k,lmax	19,14,35	19,14,35
Nref	5100	5097
Tmin,Tmax	0.747,0.886	0.680,1.000
Tmin'	0.615	

Correction method= # Reported T Limits: Tmin=0.680 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.999      Theta(max)= 26.999

R(reflections)= 0.0449( 4077)      wR2(reflections)= 0.1138( 5097)

S = 1.082      Npar= 287

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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

PLAT213_ALERT_2_C	Atom C22	has ADP max/min Ratio .....	3.3	prolat
PLAT220_ALERT_2_C	Non-Solvent Resd 1	C Ueq(max)/Ueq(min) Range	4.0	Ratio
PLAT241_ALERT_2_C	High 'MainMol'	Ueq as Compared to Neighbors of	C22	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 .....	0.00686	Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance .....		3.464	Check



#### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		2	Note
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large	10.00	Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		1	Report
PLAT793_ALERT_4_G	The Model has Chirality at Si1	(Centro SPGR)	R	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		1	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min)		2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	2	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		2	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
8 **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  
4 ALERT type 3 Indicator that the structure quality may be low  
3 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.

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

