

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) i2732

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: i2732

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Bond precision:    C-C = 0.0035 A                      Wavelength=0.71073

Cell:                      a=14.2758(6)              b=10.3266(3)              c=21.4828(9)  
                            alpha=90                      beta=99.536(3)              gamma=90

Temperature:            100 K

	Calculated	Reported
Volume	3123.2(2)	3123.2(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C28 H46 Fe Na O5 P3	?
Sum formula	C28 H46 Fe Na O5 P3	C28 H46 Fe Na O5 P3
Mr	634.40	634.40
Dx,g cm-3	1.349	1.349
Z	4	4
Mu (mm-1)	0.685	0.685
F000	1344.0	1344.0
F000'	1347.16	
h,k,lmax	17,12,26	17,12,26
Nref	5823	5814
Tmin,Tmax	0.870,0.934	0.867,0.947
Tmin'	0.837	

Correction method= # Reported T Limits: Tmin=0.867 Tmax=0.947  
AbsCorr = INTEGRATION

Data completeness= 0.998                      Theta(max)= 25.498

R(reflections)= 0.0531( 5411)              wR2(reflections)= 0.1559( 5814)

S = 1.047                      Npar= 349

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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

PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	10	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF ....		4	Note
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .		6	Check
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....		1	Check
PLAT939_ALERT_3_C	Large Value of Not (SHELXL) Weight Optimized S .	65.43	Check	
PLAT977_ALERT_2_C	Check Negative Difference Density on H3A	-0.41	eA-3	
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0	Info	



### Alert level G

PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT	Unusually Large	0.11	Report
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1	(II)	2.11	Info
PLAT960_ALERT_3_G	Number of Intensities with I <	- 2*sig(I) ...	1	Check

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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 ALERT type 2 Indicator that the structure model may be wrong or deficient  
6 ALERT type 3 Indicator that the structure quality may be low  
0 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

## 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\_PLAT911\_i2732

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PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.600 10 Report

RESPONSE: ...

;

\_vrf\_PLAT913\_i2732

;

PROBLEM: Missing # of Very Strong Reflections in FCF .... 4 Note

RESPONSE: ...

;

\_vrf\_PLAT918\_i2732

;

PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) . 6 Check

RESPONSE: ...

;

\_vrf\_PLAT934\_i2732

;

PROBLEM: Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 1 Check

RESPONSE: ...

;

\_vrf\_PLAT939\_i2732

;

PROBLEM: Large Value of Not (SHELXL) Weight Optimized S . 65.43 Check

RESPONSE: ...

;

\_vrf\_PLAT977\_i2732

;

PROBLEM: Check Negative Difference Density on H3A -0.41 eA-3

```
RESPONSE: ...  
;  
_vrf_PLAT978_i2732  
;  
PROBLEM: Number C-C Bonds with Positive Residual Density.          0 Info  
RESPONSE: ...  
;  
# end Validation Reply Form
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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 23/04/2018; check.def file version of 23/04/2018**

