

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo\_b0105\_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\_b0105\_0m

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Bond precision:    C-C = 0.0055 A                      Wavelength=0.71073

Cell:                      a=12.987(3)              b=16.187(3)              c=21.860(4)  
                            alpha=90              beta=90              gamma=90  
Temperature:              100 K

	Calculated	Reported
Volume	4595.4(16)	4595.6(16)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C46 H48 Fe2 N2 O3 Si2, C4 H10 O	C46 H48 Fe2 N2 O3 Si2, C4 H10 O
Sum formula	C50 H58 Fe2 N2 O4 Si2	C50 H58 Fe2 N2 O4 Si2
Mr	918.86	918.86
Dx,g cm-3	1.328	1.328
Z	4	4
Mu (mm-1)	0.729	0.729
F000	1936.0	1936.0
F000'	1940.00	
h,k,lmax	16,19,26	16,19,26
Nref	9026[ 5002]	8982
Tmin,Tmax	0.863,0.916	0.642,0.745
Tmin'	0.831	

Correction method= # Reported T Limits: Tmin=0.642 Tmax=0.745  
AbsCorr = MULTI-SCAN

Data completeness= 1.80/1.00                      Theta(max)= 25.999

R(reflections)= 0.0339( 8355)                      wR2(reflections)= 0.0795( 8982)

S = 1.070                                      Npar= 555

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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

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18) .....	8.98	Note
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Th(Min) ...	5	Report
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	13	Report



#### Alert level G

PLAT791_ALERT_4_G	The Model has Chirality at Si1	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G	The Model has Chirality at Si2	(Chiral SPGR)	R Verify

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
0 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  
2 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*, 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 21/06/2015; check.def file version of 21/06/2015

Datablock mo\_b0105\_0m - ellipsoid plot

