

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Moabite

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: Moabite

Bond precision:	Fe- O = 0.0042 A	Wavelength=0.71073	
Cell:	a=7.2161 (16)	b=6.4064 (15)	c=7.4706 (19)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		

	Calculated	Reported
Volume	345.36(14)	345.36(14)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	?
Moiety formula	Fe Ni O5 P	?
Sum formula	Fe Ni O5 P	Fe Ni O5 P
Mr	225.51	225.53
Dx, g cm <sup>-3</sup>	4.337	4.338
Z	4	4
Mu (mm <sup>-1</sup> )	9.998	9.998
F000	436.0	436.0
F000'	439.34	
h, k, lmax	9, 8, 10	9, 8, 10
Nref	499	499
Tmin, Tmax	0.313, 0.368	0.640, 0.746
Tmin'	0.215	

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Correction method= # Reported T Limits: Tmin=0.640 Tmax=0.746
AbsCorr = MULTI-SCAN
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Data completeness= 1.000                      Theta (max)= 28.993

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R(reflections)= 0.0328( 389)      wR2(reflections)=
S = 1.043                        0.0714( 499)
Npar= 46
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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.

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#### Alert level C

PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd	1)	2.3	Note
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4			Please Check
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.96Ang From O1	.	0.85 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.50Ang From O2	.	0.49 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.79Ang From O3	.	-0.75 eA-3

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#### Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		3	Info
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .....	(K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature .....	(K)	293	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Nil	(II)	.	1.90 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Fel	(III)	.	3.00 Info
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....		3.7	Low
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..		58.0	Degree
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....		1.649	Note
	Predicted wR2: Based on SigI**2	4.33 or SHELX Weight	6.85	

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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  
5 **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

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

