

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

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Bond precision:    C-C = 0.0103 Å

Wavelength=0.71073

Cell:                a=9.3316(16)                b=14.805(3)                c=15.010(3)  
                      alpha=109.812(3)        beta=97.307(3)        gamma=99.965(3)  
Temperature:        293 K

	Calculated	Reported
Volume	1882.5(6)	1882.5(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C21 H11 Fe N7 O), 2(C24 H20 P), H2 O	(C21 H11 Fe N7 O), (C24 H20 P), 0.5H2 O
Sum formula	C90 H64 Fe2 N14 O3 P2	C45 H32 Fe N7 O1.50 P
Mr	1563.19	781.59
Dx,g cm-3	1.379	1.379
Z	1	2
Mu (mm-1)	0.491	0.491
F000	808.0	808.0
F000'	809.14	
h,k,lmax	11,17,17	11,17,17
Nref	6638	6567
Tmin,Tmax	0.873,0.898	0.871,0.901
Tmin'	0.867	

Correction method= # Reported T Limits: Tmin=0.871 Tmax=0.901  
AbsCorr = MULTI-SCAN

Data completeness= 0.989

Theta(max)= 25.009

R(reflections)= 0.0777( 4263)

wR2(reflections)= 0.2300( 6567)

S = 1.029

Npar= 505

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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 B

PLAT420\_ALERT\_2\_B D-H Without Acceptor O1 --H101 . Please Check

**Author Response: The electronic density around the solvent O atom are somewhat weak, making it difficultly to accurately confirm the position and the direction of the H atoms bonded.**

PLAT420\_ALERT\_2\_B D-H Without Acceptor O1 --H201 . Please Check

**Author Response: The electronic density around the solvent O atom are somewhat weak, making it difficultly to accurately confirm the position and the direction of the H atoms bonded.**



### Alert level C

PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for N4 --C21 . 6.0 s.u.  
PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for N5 --C9 . 5.4 s.u.  
PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for N5 --C13 . 6.0 s.u.  
PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for C7 --C8 . 6.4 s.u.  
PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for C20 --C21 . 6.5 s.u.  
PLAT232\_ALERT\_2\_C Hirshfeld Test Diff (M-X) Fe1 --N5 . 6.3 s.u.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference N7 --C15 . 0.18 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference N7 --C16 . 0.16 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C6 --C7 . 0.17 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C7 --C12 . 0.16 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C11 --C12 . 0.19 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C19 --C20 . 0.18 Ang.  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of N7 Check  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C42 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C8 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C13 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C21 Check  
PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including O1 0.169 Check  
PLAT341\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.01027 Ang.  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 3.179 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.595 73 Report  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 1.02A From N7 0.51 eA-3  
PLAT978\_ALERT\_2\_C Number C-C Bonds with Positive Residual Density. 0 Info



### Alert level G

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 3 Note  
PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 11 Report  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 2 Report  
PLAT042\_ALERT\_1\_G Calc. and Reported MoietyFormula Strings Differ Please Check  
PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 0.50 Check  
PLAT066\_ALERT\_1\_G Predicted and Reported Tmin&Tmax Range Identical ? Check  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report  
PLAT154\_ALERT\_1\_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree  
PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 2 Report  
PLAT177\_ALERT\_4\_G The CIF-Embedded .res File Contains DELU Records 2 Report

PLAT199_ALERT_1_G	Reported _cell_measurement_temperature . . . . . (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature . . . . . (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H101 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H201 Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in . . . . . Resd 3	1.50	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (III) .	3.29	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints . . . . .	17	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	35%	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	5	Note

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

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

