

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

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Bond precision:	C-C = 0.0050 A	Wavelength=0.71073
Cell:	a=7.0270(16)	b=11.719(3)      c=15.665(4)
	alpha=77.863(13)	beta=88.928(13)      gamma=72.872(12)
Temperature:	295 K	
	Calculated	Reported
Volume	1204.0(5)	1204.0(5)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C52 H34 F4 Fe2 N4 O8, H2 O	C52 H36 F4 Fe2 N4 O9
Sum formula	C52 H36 F4 Fe2 N4 O9	C52 H36 F4 Fe2 N4 O9
Mr	1048.55	1048.56
Dx,g cm-3	1.446	1.446
Z	1	1
Mu (mm-1)	0.679	0.679
F000	536.0	536.0
F000'	536.96	
h,k,lmax	8,14,19	8,14,19
Nref	4712	4635
Tmin,Tmax	0.892,0.928	0.910,0.930
Tmin'	0.805	

Correction method= # Reported T Limits: Tmin=0.910 Tmax=0.930  
AbsCorr = NUMERICAL

Data completeness= 0.984      Theta(max)= 25.945

R(reflections)= 0.0478( 3951)      wR2(reflections)= 0.0792( 3951)

S = 1.000      Npar= 370

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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

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## Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	2	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F3 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C9 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C10 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C12 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C27 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C28 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C29 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C30 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 H121 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H131 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H281 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H291 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H301 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O5 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H331 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H332 Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	14%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 2 )	1.50	Check
PLAT769_ALERT_4_G	CIF Embedded explicitly supplied scattering data		Please Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (III) .	3.08	Info
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please Check
PLAT882_ALERT_1_G	No Datum for _diffrn_reflms_av_unetI/netI .....		Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	79	Note
PLAT929_ALERT_5_G	No Weight Pars,Obs and Calc R1,wR2,S not Checked		! Info
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	129	Check

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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  
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
31 **ALERT level G** = General information/check it is not something unexpected
- 2 **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  
23 **ALERT type 4** Improvement, methodology, query or suggestion  
4 **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.

