

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) sv0485

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: sv0485

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Bond precision:	C-C = 0.0153 A	Wavelength=1.54186
Cell:	a=10.791(1)	b=10.7753(10)      c=16.8369(16)
	alpha=73.904(7)	beta=71.663(7)      gamma=69.620(7)
Temperature:	100 K	
	Calculated	Reported
Volume	1710.8(3)	1710.8(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C30 H50 Fe K O6 P3	?
Sum formula	C30 H50 Fe K O6 P3	C30 H50 Fe K O6 P3
Mr	694.56	694.56
Dx,g cm-3	1.348	1.348
Z	2	2
Mu (mm-1)	6.265	6.265
F000	736.0	736.0
F000'	737.97	
h,k,lmax	13,13,20	13,13,20
Nref	6343	6198
Tmin,Tmax	0.534,0.882	0.451,0.887
Tmin'	0.328	

Correction method= # Reported T Limits: Tmin=0.451 Tmax=0.887  
AbsCorr = INTEGRATION

Data completeness= 0.977      Theta(max)= 68.998

R(reflections)= 0.1104( 4302)      wR2(reflections)= 0.3201( 6198)

S = 1.024      Npar= 376

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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 B

PLAT213_ALERT_2_B	Atom C20	has ADP max/min Ratio .....	4.6	prolat
PLAT234_ALERT_4_B	Large Hirshfeld Difference O2	--C21	0.26	Ang.
PLAT341_ALERT_3_B	Low Bond Precision on C-C Bonds .....		0.01532	Ang.

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### Alert level C

PLAT082_ALERT_2_C	High R1 Value .....		0.11	Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25) .....		0.32	Report
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....		2.78	Report
PLAT155_ALERT_4_C	The Triclinic Unitcell is NOT Reduced .....			Please Do !
PLAT213_ALERT_2_C	Atom C19	has ADP max/min Ratio .....	3.3	oblate
PLAT213_ALERT_2_C	Atom C21	has ADP max/min Ratio .....	3.4	prolat
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range	5.0	Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 1 H	Uiso(max)/Uiso(min) Range	5.1	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for O1	--C30	6.7	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for O5	--C26	6.3	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C27	--C28	5.6	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C29	--C30	5.4	s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference O2	--C20	0.23	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference O4	--C24	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference O6	--C28	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C19	--C20	0.25	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C21	--C22	0.22	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C25	--C26	0.19	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	O5	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C20	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C21	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C23	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C25	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	K1	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C15	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C26	Check	
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond C25	- C26	1.42	Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond C29	- C30	1.38	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	102	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .		1	Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.42A	From P1	1.68	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.92A	From Fe1	1.54	eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on	Fe1	1.26	eA-3
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.		0	Info

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### Alert level G

PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large		0.20	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		6.74	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.007	Degree
PLAT793_ALERT_4_G	Model has Chirality at P3	(Centro SPGR)		R Verify
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1	(II)	2.15	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	44	Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...		16	Check

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

3 **ALERT level B** = A potentially serious problem, consider carefully

34 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

7 **ALERT level G** = General information/check it is not something unexpected

1 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data

26 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  
 10 ALERT type 4 Improvement, methodology, query or suggestion  
 1 ALERT type 5 Informative message, check

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## 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_PLAT082_sv0485
;
PROBLEM: High R1 Value ..... 0.11 Report
RESPONSE: ...
;
_vrf_PLAT084_sv0485
;
PROBLEM: High wR2 Value (i.e. > 0.25) ..... 0.32 Report
RESPONSE: ...
;
_vrf_PLAT094_sv0485
;
PROBLEM: Ratio of Maximum / Minimum Residual Density .... 2.78 Report
RESPONSE: ...
;
_vrf_PLAT155_sv0485
;
PROBLEM: The Triclinic Unitcell is NOT Reduced ..... Please Do !
RESPONSE: ...
;
_vrf_PLAT213_sv0485
;
PROBLEM: Atom C19          has ADP max/min Ratio ..... 3.3 oblate
RESPONSE: ...
;
_vrf_PLAT220_sv0485
;
PROBLEM: Non-Solvent  Resd 1  C    Ueq(max)/Ueq(min) Range  5.0 Ratio
RESPONSE: ...
;
_vrf_PLAT222_sv0485
;
PROBLEM: Non-Solv.  Resd 1  H    Uiso(max)/Uiso(min) Range  5.1 Ratio
RESPONSE: ...
;
_vrf_PLAT230_sv0485
;
PROBLEM: Hirshfeld Test Diff for  O1      --C30      .      6.7 s.u.
RESPONSE: ...
;
_vrf_PLAT234_sv0485
;
PROBLEM: Large Hirshfeld Difference O2      --C20      0.23 Ang.
RESPONSE: ...
;
_vrf_PLAT241_sv0485
;
PROBLEM: High      'MainMol' Ueq as Compared to Neighbors of      05 Check
RESPONSE: ...
;
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\_vrf\_PLAT242\_sv0485  
;  
PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of K1 Check  
RESPONSE: ...  
;  
\_vrf\_PLAT360\_sv0485  
;  
PROBLEM: Short C(sp3)-C(sp3) Bond C25 - C26 . 1.42 Ang.  
RESPONSE: ...  
;  
\_vrf\_PLAT911\_sv0485  
;  
PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.600 102 Report  
RESPONSE: ...  
;  
\_vrf\_PLAT918\_sv0485  
;  
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) . 1 Check  
RESPONSE: ...  
;  
\_vrf\_PLAT971\_sv0485  
;  
PROBLEM: Check Calcd Resid. Dens. 1.42A From P1 1.68 eA-3  
RESPONSE: ...  
;  
\_vrf\_PLAT973\_sv0485  
;  
PROBLEM: Check Calcd Positive Resid. Density on Fe1 1.26 eA-3  
RESPONSE: ...  
;  
\_vrf\_PLAT978\_sv0485  
;  
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.

