

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

Bond precision:	C-C = 0.0232 Å	Wavelength=0.71073	
Cell:	a=13.7178(14)	b=20.452(2)	c=27.659(3)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	7759.9(14)	7759.8(14)	
Space group	P 21 21 21	P 21 21 21	
Hall group	P 2ac 2ab	P 2ac 2ab	
Moiety formula	C72 H86 Fe N6 P4, 2(B F4), 2(C2 H3 N)	C72 H86 Fe N6 P4, 2(B F4), 2(C2 H3 N)	
Sum formula	C76 H92 B2 F8 Fe N8 P4	C76 H92 B2 F8 Fe N8 P4	
Mr	1470.93	1470.92	
Dx, g cm ⁻³	1.259	1.259	
Z	4	4	
Mu (mm ⁻¹)	0.342	0.342	
F000	3088.0	3088.0	
F000'	3092.27		
h,k,lmax	16,25,33	16,24,33	
Nref	14986[8195]	14690	
Tmin,Tmax	0.960,0.983	0.619,0.746	
Tmin'	0.934		

Correction method= # Reported T Limits: Tmin=0.619 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.79/0.98 Theta(max)= 25.842

R(reflections)= 0.0791(7289) wR2(reflections)= 0.2081(14690)

S = 1.007 Npar= 866

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

RINTA01_ALERT_3_B The value of Rint is greater than 0.18

Rint given 0.197

PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 0.197 Report

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.02317 Ang.

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 15 Note

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

PLAT213_ALERT_2_C Atom C13 has ADP max/min Ratio 3.1 prolat

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max) / Ueq(min) Range 4.6 Ratio

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.6 Ratio

PLAT234_ALERT_4_C Large Hirshfeld Difference C33B --C34B . 0.18 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C36 --C37 . 0.19 Ang.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C13 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C13B Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C26B Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C29 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C36B Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C18B Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C24B Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C33B Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C41 Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C51 Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C61 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including F1 0.211 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including F5 0.265 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including N50 0.162 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including N60 0.182 Check

PLAT332_ALERT_2_C Large Phenyl C-C Range C26B -C31B . 0.20 Ang.

PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 37 Ang**3

PLAT761_ALERT_1_C CIF Contains no X-H Bonds Please Check

PLAT762_ALERT_1_C CIF Contains no X-Y-H or H-Y-H Angles Please Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 5 Note

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 10.32 Why ?

PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report

PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 4 Report

PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of B1 Check

PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of B2 Check

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 8 Note

PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #
C2 H3 N 5 Note

PLAT791_ALERT_4_G Model has Chirality at P3B (Sohnke SpGr) R Verify

PLAT791_ALERT_4_G Model has Chirality at P7B (Sohnke SpGr) S Verify

PLAT791_ALERT_4_G Model has Chirality at C9 (Sohnke SpGr) R Verify

PLAT791_ALERT_4_G Model has Chirality at C9B (Sohnke SpGr) R Verify

PLAT791_ALERT_4_G Model has Chirality at C24 (Sohnke SpGr) R Verify

PLAT791_ALERT_4_G Model has Chirality at C24B (Sohnke SpGr) R Verify

PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	4	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	92	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	17	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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

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

checkCIF publication errors

Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
 _publ_contact_author_name and _publ_contact_author_address.
 PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
 _publ_contact_author_phone are all missing.
 At least one of these should be present.
 PUBL006_ALERT_1_A _publ_requested_journal is missing
 e.g. 'Acta Crystallographica Section C'
 PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
 PUBL012_ALERT_1_A _publ_section_abstract is missing.
 Abstract of paper in English.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or
 empty.

5 **ALERT level A** = Data missing that is essential or data in wrong format
 1 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

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_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 22/04/2020; check.def file version of 09/03/2020

Datablock I - ellipsoid plot

