

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 11

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: 11

Bond precision:	C-C = 0.0084 Å	Wavelength=0.71073
Cell:	a=12.7531(6)	b=8.4120(4) c=25.2975(10)
	alpha=90	beta=96.017(4) gamma=90
Temperature:	297 K	
	Calculated	Reported
Volume	2698.9(2)	2698.9(2)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C48 H54 Au2 N10, 2(F6 P)	C48 H54 Au2 N10, 2(F6 P)
Sum formula	C48 H54 Au2 F12 N10 P2	C48 H54 Au2 F12 N10 P2
Mr	1454.89	1454.88
Dx,g cm-3	1.790	1.790
Z	2	2
Mu (mm-1)	5.574	5.574
F000	1416.0	1416.0
F000'	1409.29	
h,k,lmax	15,10,31	15,10,31
Nref	5521	5514
Tmin,Tmax	0.381,0.800	0.372,1.000
Tmin'	0.181	

Correction method= # Reported T Limits: Tmin=0.372 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 26.367

R(reflections)= 0.0330(4847) wR2(reflections)= 0.0818(5514)

S = 1.093 Npar= 338

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.40	Report
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including P1	0.105	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0084	Ang.
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
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.062	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	4	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.91A From Aul	2.31	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.83A From Aul	2.07	eA-3

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	7	Report
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF		Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	7.24	Why ?
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	P1	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	63	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	4	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 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
2 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.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

7 **ALERT level A** = Data missing that is essential or data in wrong format
0 **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_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
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 18/02/2019; check.def file version of 18/02/2019

Datablock 11 - ellipsoid plot

