

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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 = 0.0064 A	Wavelength=0.71073
Cell:	a=9.2691(5)	b=19.1597(8) c=19.6184(10)
	alpha=86.078(4)	beta=76.950(5) gamma=88.752(4)
Temperature:	130 K	
	Calculated	Reported
Volume	3386.1(3)	3386.1(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C34 H49 Au F3 P S	C34 H49 Au F3 P S
Sum formula	C34 H49 Au F3 P S	C34 H49 Au F3 P S
Mr	774.73	774.73
Dx,g cm-3	1.520	1.520
Z	4	4
Mu (mm-1)	4.491	4.491
F000	1560.0	1560.0
F000'	1553.63	
h,k,lmax	12,26,27	12,24,27
Nref	18953	15838
Tmin,Tmax	0.321,0.481	0.347,0.535
Tmin'	0.081	

Correction method= # Reported T Limits: Tmin=0.347 Tmax=0.535
AbsCorr = ANALYTICAL

Data completeness= 0.836 Theta(max)= 29.544

R(reflections)= 0.0373(12323) wR2(reflections)= 0.0845(15838)

S = 1.026 Npar= 734

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

PLAT230_ALERT_2_B Hirshfeld Test Diff for S5 --C40B . 8.3 s.u.

Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 3.2 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C17B Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C33 Check
PLAT303_ALERT_2_C Full Occupancy Atom H10B with # Connections 1.34 Check
PLAT480_ALERT_4_C Long H...A H-Bond Reported H19 ..F1B . 2.61 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H13B ..F2 . 2.62 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H19 ..F1B . 2.61 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H13B ..F2 . 2.62 Ang.

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 8 Report
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT230_ALERT_2_G Hirshfeld Test Diff for C7B --C12B . 7.5 s.u.
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C40B Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C39 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 10% Note
PLAT410_ALERT_2_G Short Intra H...H Contact H9BA ..H10A . 1.97 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H9BA ..H10B . 1.65 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H11A ..H12A . 1.96 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H11A ..H12D . 2.03 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H11B ..H12D . 2.06 Ang.
x,y,z = 1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 8 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 376 Check
C10B -C9P -H10B 1.555 1.555 1.555 33.50 Deg.
PLAT793_ALERT_4_G Model has Chirality at C7B (Centro SPGR) R Verify
PLAT793_ALERT_4_G Model has Chirality at C7P (Centro SPGR) S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints 55 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 2 Units

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

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

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or
empty.

7 **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
```

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;
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 05/12/2020; check.def file version of 05/12/2020

