

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) LOL149AS

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: LOL149AS

Bond precision: C-C = 0.0151 Å

Wavelength=0.71073

Cell: a=12.538(4) b=12.721(4) c=17.645(5)
 alpha=69.941(5) beta=81.474(5) gamma=89.259(5)
Temperature: 100 K

	Calculated	Reported
Volume	2612.2(14)	2612.1(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C23 H21 Au N4 O P S2, C23 H22 Au N4 O P S2, C H2 Cl2	? ?
Sum formula	C47 H45 Au2 Cl2 N8 O2 P2 S4	C47 H45 Au2 Cl2 N8 O2 P2 S4
Mr	1408.93	1408.92
Dx, g cm ⁻³	1.791	1.791
Z	2	2
Mu (mm ⁻¹)	5.979	5.979
F000	1370.0	1370.0
F000'	1364.57	
h,k,lmax	15,15,21	15,15,21
Nref	10265	10187
Tmin,Tmax	0.427,0.787	0.328,0.591
Tmin'	0.236	

Correction method= # Reported T Limits: Tmin=0.328 Tmax=0.591
AbsCorr = MULTI-SCAN

Data completeness= 0.992

Theta(max)= 26.000

R(reflections)= 0.0556(7887)

wR2(reflections)= 0.1376(10187)

S = 1.012

Npar= 600

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 A

PLAT971_ALERT_2_A	Check Calcd Resid. Dens.	0.98A	From Au1	4.18 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens.	1.03A	From Au2	4.17 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens.	1.10A	From Au1	3.89 eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens.	1.08A	From Au2	3.70 eA-3

Alert level B

PLAT201_ALERT_2_B	Isotropic non-H Atoms in Main Residue(s)	2 Report
PLAT971_ALERT_2_B	Check Calcd Resid. Dens.	0.88A From Au1 3.28 eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens.	0.92A From Au2 3.24 eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens.	0.96A From Au2 3.03 eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens.	0.99A From Au2 3.01 eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens.	0.93A From Au1 2.86 eA-3

Alert level C

PLAT048_ALERT_1_C	MoietyFormula Not Given (or Incomplete)	Please Check
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.53 Report
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.2 Ratio
PLAT220_ALERT_2_C	Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range	3.2 Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C34 Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01508 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	4.247 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	42 Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.90A From Au2 2.40 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.94A From C55 -1.73 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.26A From C100 -1.52 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H3B	-0.32 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H33	-0.31 eA-3
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0 Info

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	4 Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	6 Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.005 Degree
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	6% Note
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C31 --C32	1.76 Ang.
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	34 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1 Note

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

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

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

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

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

23 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

1 ALERT type 4 Improvement, methodology, query or suggestion

1 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.

```
# 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: ...
;
_vrf_PLAT971_LOL149AS
;
PROBLEM: Check Calcd Resid. Dens.  0.98A    From Aul          4.18 eA-3
RESPONSE: ...
;
# end Validation Reply Form

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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 19/10/2018; check.def file version of 15/10/2018

