# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mob639

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: mob639

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Bond precision: C-C = 0.0043 A Wavelength=0.71073

Cell: a=10.8581(4) b=12.6003(6) c=12.9796(5)
alpha=72.307(4) beta=89.235(3) gamma=71.190(4)
Temperature: 150 K

| | Calculated | Reported |
|---|---|---|
| Volume | 1594.39(13) | 1594.39(12) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C48 H60 Ag4 N16 O8, 10(H2 O) | C48 H60 Ag4 N16 O8, 10(H2 O) |
| Sum formula | C48 H80 Ag4 N16 O18 | C48 H80 Ag4 N16 O18 |
| Mr | 1600.76 | 1600.76 |
| Dx,g cm-3 | 1.667 | 1.667 |
| Z | 1 | 1 |
| Mu (mm-1) | 1.288 | 1.288 |
| F000 | 812.0 | 812.0 |
| F000’ | 808.73 | |
| h,k,lmax | 15,17,18 | 14,17,17 |
| Nref | 9663 | 8314 |
| Tmin,Tmax | 0.635,0.679 | 0.540,1.000 |
| Tmin’ | 0.591 | |

Correction method= # Reported T Limits: Tmin=0.540 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.860 Theta(max)= 30.414

R(reflections)= 0.0340( 6539) wR2(reflections)= 0.0763( 8314)

S = 1.060 Npar= 406

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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 C**

PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 5 Note
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.97A From N3 0.54 eA-3

**Author Response: This residual density peak is not chemically reasonable and does not represent the real atom.**

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**Alert level G**

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 10 Report

**Author Response: Positions of hydrogens on water molecules were obtained from difference electron density map. Due to unstable refinement, they were further treated with AFIX 3 command riding on their carrier oxygens.**

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ag1 --N7 . 8.5 s.u.
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C12 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 10 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 5 Note
H2 O
PLAT793_ALERT_4_G Model has Chirality at C14 (Centro SPGR) S Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 1248 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 1.8 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

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

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# checkCIF publication errors

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**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

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            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.
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### Alert level G

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PUBL017_ALERT_1_G The _publ_section_references section is missing or
            empty.
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   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
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**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
;
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.

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**PLATON version of 22/03/2021; check.def file version of 19/03/2021**

**Datablock mob639** - ellipsoid plot