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 = 0.0079 A              Wavelength=0.71073

Cell:              a=20.3981(4)      b=20.3981(4)        c=12.9725(3)
                   alpha=90          beta=90             gamma=120
Temperature:       123 K

                   Calculated                   Reported
Volume             4674.5(2)                    4674.5(2)
Space group        P -3                         P -3
Hall group         -P 3                         -P 3
                                                C30 H45 Ag1 As15 Fe3, Al1
                   C36 Al F46 O3, C30 H45 Ag
Moiety formula                                  C36 F46 O3, 0.33(C3 H6
                   As15 Fe3, C H2 Cl2
                                                Cl6)
                   C67 H47 Ag Al As15 Cl2 F46  C67 H47 Ag Al As15 Cl2 F46
Sum formula
                   Fe3 O3                       Fe3 O3
Mr                 3271.10                      3271.14
Dx,g cm-3          2.324                        2.324
Z                  2                            2
Mu (mm-1)          6.135                        6.135
F000               3108.0                       3108.0
F000'              3112.53
h,k,lmax           25,25,16                     25,25,16
Nref               6386                         6246
Tmin,Tmax          0.414,0.545                  0.257,0.639
Tmin'              0.095

Correction method= # Reported T Limits: Tmin=0.257 Tmax=0.639
AbsCorr = GAUSSIAN

Data completeness= 0.978          Theta(max)= 26.368

R(reflections)= 0.0318( 4448)     wR2(reflections)= 0.0859( 6246)

S = 0.948                    Npar= 432
```

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

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low ....   0.978 Note

⬤ Alert level G

```
FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and _chemical_formula_moiety. This is
            usually due to the moiety formula being in the wrong format.
            Atom count from _chemical_formula_sum:   C67 H47 Ag1 Al1 As15 Cl2 F4
            Atom count from _chemical_formula_moiety:C66.99 H46.98 Ag1 Al1 As15
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       3 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       1 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ   Please Check
PLAT169_ALERT_4_G The CIF-Embedded .res File Contains AFIX 1 Recds       2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       1 Report
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   Cl1    -- C23     ..      6.0 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  As1    -- Fe1     ..      5.3 su
PLAT300_ALERT_4_G Atom Site Occupancy of <Cl2    is Constrained at    0.333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C23    is Constrained at    0.333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Cl2_c  is Constrained at    0.333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C23_c  is Constrained at    0.333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Cl2_d  is Constrained at    0.333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C23_d  is Constrained at    0.333 Check
PLAT302_ALERT_4_G Anion/Solvent Disorder ............ Percentage =       67 Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....      C8 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #       4 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       8 Note
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   1 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

   2 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
   2 ALERT type 3 Indicator that the structure quality may be low
  12 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

checkCIF publication errors

⬤ Alert level A

```
PUBL002_ALERT_1_A  The contact author's address is missing,
            _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_PUBL002_GLOBAL
;
PROBLEM: The contact author's address is 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 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 29/01/2015; check.def file version of 29/01/2015

Datablock I - ellipsoid plot