

# 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

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|                 |   |   |
|-----------------|---|---|
| Bond precision: | C-C = 0.0055 A  | Wavelength=1.54184                                      |
| Cell:           | a=23.46603(13)      b=19.73024(9)      c=34.51847(19)     |   |
|                 | alpha=90      beta=108.1596(6)      gamma=90              |   |
| Temperature:    | 123 K   |   |
|                 | Calculated  | Reported  |
| Volume          | 15185.70(15)  | 15185.70(15)  |
| Space group     | P 21/n  | P 1 21/n 1  |
| Hall group      | -P 2yn  | -P 2yn  |
| Moiety formula  | C80 H120 Ag4 Fe8 P40,<br>4(C36 Al F46 O3), 2(C H2<br>Cl2) | C80 H120 Ag4 Fe8 P40, 4(Al<br>C36 F46 O3), 2(C1 H2 Cl2) |
| Sum formula     | C226 H124 Ag4 Al4 Cl4 F184<br>Fe8 O12 P40                 | C226 H124 Ag4 Al4 Cl4 F184<br>Fe8 O12 P40               |
| Mr              | 8894.06   | 8894.04   |
| Dx,g cm-3       | 1.945   | 1.945   |
| Z               | 2   | 2   |
| Mu (mm-1)       | 8.976   | 8.976   |
| F000            | 8696.0  | 8696.0  |
| F000'           | 8743.70   |   |
| h,k,lmax        | 27,23,41  | 27,23,41  |
| Nref            | 26862   | 26626   |
| Tmin,Tmax       | 0.386,0.655   | 0.473,0.699   |
| Tmin'           | 0.292   |   |

Correction method= # Reported T Limits: Tmin=0.473 Tmax=0.699  
AbsCorr = GAUSSIAN

Data completeness= 0.991      Theta(max)= 66.656

R(reflections)= 0.0338( 16605)      wR2(reflections)= 0.0690( 26626)

S = 0.783      Npar= 2212

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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 B**

PLAT019\_ALERT\_1\_B [\\_diffrn\\_measured\\_fraction\\_theta\\_full/\\_max < 1.0](#) 0.978 Report

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**Alert level C**

GOODF01\_ALERT\_2\_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00

Goodness of fit given = 0.783

PLAT220\_ALERT\_2\_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 3.7 Ratio  
PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for P12 -- P13 .. 5.1 su  
PLAT241\_ALERT\_2\_C High Ueq as Compared to Neighbors for ..... P11 Check

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**Alert level G**

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 6 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  
PLAT142\_ALERT\_4\_G su on b - Axis Small or Missing ..... 0.00009 Ang.  
PLAT143\_ALERT\_4\_G su on c - Axis Small or Missing ..... 0.00019 Ang.  
PLAT176\_ALERT\_4\_G The CIF-Embedded .res File Contains SADI Records 2 Report  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Ag1 -- P1 .. 17.4 su  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Ag1 -- P11 .. 19.1 su  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Ag1 -- P4\_a .. 12.0 su  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Fe1 -- P5 .. 5.3 su  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Fe3 -- P12 .. 5.3 su  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Fe3 -- C25 .. 5.5 su  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of >C13 is Constrained at 0.560 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of >C14 is Constrained at 0.560 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of >C901 is Constrained at 0.560 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of <C11 is Constrained at 0.440 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of <C12 is Constrained at 0.440 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of <C900 is Constrained at 0.440 Check  
PLAT302\_ALERT\_4\_G Anion/Solvent Disorder ..... Percentage = 100 Note  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms ( 2.80) in Resd. # 4 Check  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms ( 2.20) in Resd. # 5 Check  
PLAT328\_ALERT\_4\_G Possible Missing H on sp3? Phosphorus ..... P2 Check  
PLAT328\_ALERT\_4\_G Possible Missing H on sp3? Phosphorus ..... P5 Check  
PLAT328\_ALERT\_4\_G Possible Missing H on sp3? Phosphorus ..... P9 Check  
PLAT328\_ALERT\_4\_G Possible Missing H on sp3? Phosphorus ..... P10 Check  
PLAT328\_ALERT\_4\_G Possible Missing H on sp3? Phosphorus ..... P13 Check  
PLAT328\_ALERT\_4\_G Possible Missing H on sp3? Phosphorus ..... P14 Check  
PLAT328\_ALERT\_4\_G Possible Missing H on sp3? Phosphorus ..... P15 Check  
PLAT328\_ALERT\_4\_G Possible Missing H on sp3? Phosphorus ..... P17 Check  
PLAT328\_ALERT\_4\_G Possible Missing H on sp3? Phosphorus ..... P18 Check  
PLAT328\_ALERT\_4\_G Possible Missing H on sp3? Phosphorus ..... P19 Check  
PLAT328\_ALERT\_4\_G Possible Missing H on sp3? Phosphorus ..... P20 Check  
PLAT380\_ALERT\_4\_G Incorrectly? Oriented X(sp2)-Methyl Moiety .... C17 Check  
PLAT380\_ALERT\_4\_G Incorrectly? Oriented X(sp2)-Methyl Moiety .... C39 Check  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact P8 .. P19 .. 3.35 Ang.  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact F43 .. C31 .. 2.89 Ang.  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact F89 .. C2 .. 2.89 Ang.  
PLAT434\_ALERT\_2\_G Short Inter HL..HL Contact F9 .. F67 .. 2.82 Ang.  
PLAT434\_ALERT\_2\_G Short Inter HL..HL Contact F22 .. F51 .. 2.83 Ang.  
PLAT434\_ALERT\_2\_G Short Inter HL..HL Contact F24 .. F53 .. 2.80 Ang.  
PLAT434\_ALERT\_2\_G Short Inter HL..HL Contact F35 .. F60 .. 2.81 Ang.

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

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

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## checkCIF publication errors

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### 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.

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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

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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.

## 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.

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**PLATON version of 29/01/2015; check.def file version of 29/01/2015**

