# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) P-1_a

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: P-1_a

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```
Bond precision:   C-C = 0.0037 A           Wavelength=0.71073

Cell:           a=13.559(5)        b=18.467(4)        c=19.117(4)
                alpha=85.951(7)    beta=84.779(13)    gamma=86.198(5)
Temperature:    100 K
```

| | Calculated | Reported |
|---|---|---|
| Volume | 4746(2) | 4746(2) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C16 Al F36 O4, C57 H60 Al3 P2, C10 H15 Al, C6 H4 F2 | [AL(C37H30P2)AL3(C10H15)3][ALO4C16F36]_C6H4F2 |
| Sum formula | C89 H79 Al5 F38 O4 P2 | C89 O4 F38 Al5 P2 H79 |
| Mr | 2131.36 | 2131.40 |
| Dx,g cm-3 | 1.492 | 1.491 |
| Z | 2 | 2 |
| Mu (mm-1) | 0.216 | 0.216 |
| F000 | 2164.0 | 2164.0 |
| F000' | 2166.75 | |
| h,k,lmax | 16,22,23 | 16,22,23 |
| Nref | 18792 | 18769 |
| Tmin,Tmax | 0.956,0.975 | 0.708,0.745 |
| Tmin' | 0.953 | |

```
Correction method= # Reported T Limits: Tmin=0.708 Tmax=0.745
AbsCorr = MULTI-SCAN
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Data completeness= 0.999 Theta(max)= 26.058

R(reflections)= 0.0436( 13990) wR2(reflections)= 0.1147( 18769)

S = 1.019 Npar= 1808

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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

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT213_ALERT_2_C Atom F8_8 has ADP max/min Ratio ..... 3.5 prolat
PLAT220_ALERT_2_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 3.4 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C3 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.1 Note
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C1_2 -C6_2 1.36 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report

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## 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: C89 H79 Al5 F38 O4 P2
Atom count from _chemical_formula_moiety:
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 120 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 134 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ Please Check
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 2 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 3 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 15 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 9 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 8 Report
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C02C Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C02E Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C02K Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1 ) 74% Note
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 2 ) 16% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4 ) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5 ) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 4 ) 9.95 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 5 ) 2.05 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H48C ..H10A_4 . 1.87 Ang.
x,y,z = 1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F00A ..F1_2 2.74 Ang.
x,1+y,z = 1_565 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 175 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 8733 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 22 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 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
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  25 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
  11 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.
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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
```

**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 18/12/2021; check.def file version of 18/12/2021**

**Datablock P-1_a** - ellipsoid plot