checkCIF/PLATON report

Structure factors have been supplied for datablock(s) P21c_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: P21c_a

```
Bond precision:   C-C = 0.0030 A          Wavelength=0.71073

Cell:             a=16.361(4)     b=32.286(10)          c=18.454(4)
                  alpha=90        beta=109.236(10)      gamma=90
Temperature:      100 K
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	Calculated	Reported
Volume	9204(4)	9204(4)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C16 Al F36 O4, C30 H45 Al3, C21 H30 Al N6, 0.664(C6 H4 F2), 0.8 C75.10 H86.72	[(DMAP)3AL(ALCP*)3][AL(OC4F9)4]
Sum formula	Al5 F37.33 N6 O4	C75.10 H86.72 Al5 F37.33 N6 O4
Mr	1981.60	1981.57
Dx,g cm-3	1.430	1.430
Z	4	4
Mu (mm-1)	0.184	0.184
F000	4049.2	4049.0
F000'	4053.71	
h,k,lmax	20,40,23	20,40,23
Nref	18899	18867
Tmin,Tmax	0.957,0.975	0.711,0.745
Tmin'	0.939	

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Correction method= # Reported T Limits: Tmin=0.711 Tmax=0.745
AbsCorr = MULTI-SCAN
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Data completeness= 0.998 Theta(max)= 26.405

R(reflections)= 0.0413(14979) wR2(reflections)= 0.1174(18867)

S = 1.030 Npar= 1978

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

PLAT088_ALERT_3_C Poor Data / Parameter Ratio ..... 9.54 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.76 Report
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C1_6 0.102 Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C1_24 -C6_24 1.36 Ang.
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C1_23 -C6_23 1.36 Ang.
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of . 62 Ang**3
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 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: C75.1 H86.72 Al5 F37.33 N6 O4
Atom count from _chemical_formula_moiety:
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 201 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 201 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ Please Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.65 Why ?
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 3 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 5 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 21 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 14 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 13 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 98% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 61% 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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 4) 3.26 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 5) 4.70 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 6) 13.18 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C6_10 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C6_21 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H5_8 ..H7B_22 . 2.09 Ang.
x,y,z = 1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 307 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 4 Note
C6 H4 F2
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 6 Note
C5 H11

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PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      16307 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         25 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          9 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          4 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
  32 **ALERT level G** = General information/check it is not something unexpected

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

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checkCIF publication errors

Alert level A

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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

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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.

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

Datablock P21c_a - ellipsoid plot