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 = 0.0061 A          Wavelength=1.54184

Cell:          a=36.3787(4)   b=16.16213(17)       c=14.51853(16)
               alpha=90       beta=101.5137(10)    gamma=90
Temperature:   123 K
```

	Calculated	Reported
Volume	8364.50(16)	8364.49(16)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C16 Al F36 O4, C40 H60 Ag Mo4 P12, C0.43 H0.86 Cl0.86, 2(C0.28	Al C16 F36 O4, C40 H60 Ag Mo4 P12, 3.45(C0.29 H0.58 Cl0.58)
Sum formula	C57 H62 Ag Al Cl2 F36 Mo4 O4 P12	C57 H62 Ag Al Cl2 F36 Mo4 O4 P12
Mr	2456.22	2456.21
Dx,g cm-3	1.951	1.950
Z	4	4
Mu (mm-1)	10.624	10.624
F000	4808.0	4808.0
F000’	4841.02	
h,k,lmax	45,20,18	45,19,17
Nref	8442	8226
Tmin,Tmax	0.439,0.516	0.435,0.617
Tmin’	0.271	

```
Correction method= # Reported T Limits: Tmin=0.435 Tmax=0.617
AbsCorr = GAUSSIAN

Data completeness= 0.974          Theta(max)= 73.708

R(reflections)= 0.0413( 7474)     wR2(reflections)= 0.1167( 8226)

S = 1.067                 Npar= 738
```

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 B

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ..... 4 Report

Author Response: 4 atoms of a disordered tert-butyl group with 51% occupancy were kept isotropic during the refinement. Otherwise the displacement parameters of these atoms adopted very unrealistic values.

PLAT213_ALERT_2_B Atom F29 has ADP max/min Ratio ..... 4.4 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_B Atom F34 has ADP max/min Ratio ..... 4.5 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_B Atom F36 has ADP max/min Ratio ..... 4.2 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_B Atom C56 has ADP max/min Ratio ..... 4.6 oblate

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) Range 6.9 Ratio

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

Alert level C

PLAT213_ALERT_2_C Atom F19 has ADP max/min Ratio ..... 3.9 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_C Atom F21 has ADP max/min Ratio ..... 3.7 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_C Atom F27 has ADP max/min Ratio ..... 3.2 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_C Atom F4 has ADP max/min Ratio ..... 3.2 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_C Atom F7 has ADP max/min Ratio ..... 3.3 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_C Atom F9 has ADP max/min Ratio ..... 3.2 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_C Atom F32 has ADP max/min Ratio ..... 3.1 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT213_ALERT_2_C Atom C52 has ADP max/min Ratio ..... 3.5 prolat

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT220_ALERT_2_C Large Non-Solvent F Ueq(max)/Ueq(min) Range 3.6 Ratio

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion.

PLAT234_ALERT_4_C Large Hirshfeld Difference C49 -- C50 .. 0.25 Ang.

Author Response: The weakly coordinating aluminate anion exhibits disorder and a large degree of thermal motion. The ternary C atom of the tert-butyl groups are not as heavily concerned by the motion.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... Al4 Check

Author Response: Al is the central atom of a heavily disordered anion with large displacement parameters.

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 ... 4 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 36.36 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 4 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 36 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for F25 -- C52 .. 6.2 su
PLAT230_ALERT_2_G Hirshfeld Test Diff for F27 -- C52 .. 5.6 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo1 -- P2 .. 5.4 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo1 -- P3 .. 5.4 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo1 -- P4 .. 6.0 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo1 -- P5 .. 5.2 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo1 -- P6 .. 6.8 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo2 -- P1 .. 6.0 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo2 -- P2 .. 5.2 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo2 -- P3 .. 5.4 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo2 -- P4 .. 5.4 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo2 -- P5 .. 6.4 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mo2 -- P6 .. 6.4 su
PLAT300_ALERT_4_G Atom Site Occupancy of >F10 is Constrained at 0.511 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F11 is Constrained at 0.511 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F12 is Constrained at 0.511 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F13 is Constrained at 0.511 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F14 is Constrained at 0.511 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F15 is Constrained at 0.511 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F16 is Constrained at 0.511 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F17 is Constrained at 0.511 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F18 is Constrained at 0.511 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F19 is Constrained at 0.515 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F20 is Constrained at 0.515 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F21 is Constrained at 0.515 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F22 is Constrained at 0.515 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F23 is Constrained at 0.515 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F24 is Constrained at 0.515 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F25 is Constrained at 0.515 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F26 is Constrained at 0.515 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F27 is Constrained at 0.515 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >O2 is Constrained at 0.511 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >O3 is Constrained at 0.515 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F1 is Constrained at 0.489 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F2 is Constrained at 0.489 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F3 is Constrained at 0.489 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F4 is Constrained at 0.489 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F5 is Constrained at 0.489 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F6 is Constrained at 0.489 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F7 is Constrained at 0.489 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F8 is Constrained at 0.489 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F9 is Constrained at 0.489 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F28 is Constrained at 0.485 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of <F29    is Constrained at      0.485 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F30    is Constrained at      0.485 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F31    is Constrained at      0.485 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F32    is Constrained at      0.485 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F33    is Constrained at      0.485 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F34    is Constrained at      0.485 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F35    is Constrained at      0.485 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F36    is Constrained at      0.485 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <O1     is Constrained at      0.489 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <O4     is Constrained at      0.485 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C45    is Constrained at      0.511 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C46    is Constrained at      0.511 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C47    is Constrained at      0.511 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C48    is Constrained at      0.511 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C49    is Constrained at      0.515 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C50    is Constrained at      0.515 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C51    is Constrained at      0.515 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C52    is Constrained at      0.515 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C41    is Constrained at      0.489 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C42    is Constrained at      0.489 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C43    is Constrained at      0.489 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C44    is Constrained at      0.489 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C53    is Constrained at      0.485 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C54    is Constrained at      0.485 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C55    is Constrained at      0.485 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C56    is Constrained at      0.485 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Cl1    is Constrained at      0.430 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C500   is Constrained at      0.430 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H50C   is Constrained at      0.215 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H50D   is Constrained at      0.215 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Cl2    is Constrained at      0.290 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C501   is Constrained at      0.290 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H50A   is Constrained at      0.145 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H50B   is Constrained at      0.145 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Cl3    is Constrained at      0.280 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C502   is Constrained at      0.280 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H50E   is Constrained at      0.140 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H50F   is Constrained at      0.140 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =         49 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =        100 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   2.15) in Resd. #          3 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   1.45) in Resd. #          4 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   1.40) in Resd. #          5 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C9 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C16 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C20 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        109 Note
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  0 ALERT level A = Most likely a serious problem - resolve or explain
  6 ALERT level B = A potentially serious problem, consider carefully
 11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
100 ALERT level G = General information/check it is not something unexpected

  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 32 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
 81 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

```
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 21/06/2015; check.def file version of 21/06/2015

Datablock I - ellipsoid plot