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 = 0.0070 A          Wavelength=1.54180

Cell:           a=36.4679(6)    b=16.1466(3)        c=14.4134(2)
                alpha=90        beta=101.863(2)     gamma=90
Temperature:    123 K
```

	Calculated	Reported
Volume	8305.8(2)	8305.8(2)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C16 Al F36 O4, C40 H60 Cu Mo4 P12, C H2 Cl2	C40 H60 Cu Mo4 P12, Al C16 F36 O4, C1 H2 Cl2
Sum formula	C57 H62 Al Cl2 Cu F36 Mo4 O4 P12	C57 H62 Al Cl2 Cu F36 Mo4 O4 P12
Mr	2411.90	2411.88
Dx,g cm-3	1.929	1.929
Z	4	4
Mu (mm-1)	9.123	9.123
F000	4736.0	4736.0
F000’	4760.32	
h,k,lmax	43,19,17	43,19,17
Nref	7598	7599
Tmin,Tmax	0.141,0.397	0.187,0.509
Tmin’	0.032	

```
Correction method= # Reported T Limits: Tmin=0.187 Tmax=0.509
AbsCorr = ANALYTICAL

Data completeness= 1.000          Theta(max)= 68.238

R(reflections)= 0.0472( 7558)     wR2(reflections)= 0.1090( 7599)

S = 1.112                 Npar= 758
```

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

PLAT213_ALERT_2_B Atom F33 has ADP max/min Ratio ..... 4.2 oblate

Author Response: The weakly coordinating aluminate anion exhibits strong thermal \ motion. The terminal fluorine atoms are strongly affected by this.

Alert level C

PLAT213_ALERT_2_C Atom F17 has ADP max/min Ratio ..... 3.2 prolat

Author Response: The weakly coordinating aluminate anion exhibits strong thermal \ motion. The terminal fluorine atoms are strongly affected by this.

PLAT213_ALERT_2_C Atom F10 has ADP max/min Ratio ..... 3.9 prolat

Author Response: The weakly coordinating aluminate anion exhibits strong thermal \ motion. The terminal fluorine atoms are strongly affected by this.

PLAT213_ALERT_2_C Atom F27 has ADP max/min Ratio ..... 3.1 prolat

Author Response: The weakly coordinating aluminate anion exhibits strong thermal \ motion. The terminal fluorine atoms are strongly affected by this.

PLAT213_ALERT_2_C Atom F36 has ADP max/min Ratio ..... 3.3 prolat

Author Response: The weakly coordinating aluminate anion exhibits strong thermal \ motion. The terminal fluorine atoms are strongly affected by this.

PLAT213_ALERT_2_C Atom F38 has ADP max/min Ratio ..... 3.8 prolat

Author Response: The weakly coordinating aluminate anion exhibits strong thermal \ motion. The terminal fluorine atoms are strongly affected by this.

PLAT213_ALERT_2_C Atom C29 has ADP max/min Ratio ..... 3.3 prolat

Author Response: The weakly coordinating aluminate anion exhibits strong thermal \ motion. The terminal fluorine atoms are strongly affected by this.

PLAT214_ALERT_2_C Atom Cl1 (Anion/Solvent) ADP max/min Ratio 4.4 prolat
PLAT220_ALERT_2_C Large Non-Solvent F Ueq(max)/Ueq(min) Range 3.2 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference F2 -- C22 .. 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F5 -- C23 .. 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F7 -- C24 .. 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F17 -- C28 .. 0.17 Ang.

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PLAT234_ALERT_4_C Large Hirshfeld Difference F18    --  C28     ..       0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F30    --  C26     ..       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C21    --  C30     ..       0.18 Ang.
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        Al1 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C21 Check
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Alert level G

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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 ...         7 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.     100.83 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records        11 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F31    --  C26     ..        6.8 su
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F32    --  C26     ..        7.1 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo1    --  P2      ..        6.0 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo2    --  P1      ..        6.2 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo2    --  P2      ..        5.3 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo2    --  P6      ..        5.5 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1    --  P1      ..        5.1 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1    --  P2      ..        7.5 su
PLAT300_ALERT_4_G Atom Site Occupancy of >F1     is Constrained at      0.527 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F2     is Constrained at      0.527 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F3     is Constrained at      0.527 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F4     is Constrained at      0.527 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F5     is Constrained at      0.527 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F6     is Constrained at      0.527 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F7     is Constrained at      0.527 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F8     is Constrained at      0.527 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F9     is Constrained at      0.527 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F13    is Constrained at      0.520 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F14    is Constrained at      0.520 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F15    is Constrained at      0.520 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F16    is Constrained at      0.520 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F17    is Constrained at      0.520 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F18    is Constrained at      0.520 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F30    is Constrained at      0.520 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F31    is Constrained at      0.520 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F32    is Constrained at      0.520 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >O2     is Constrained at      0.527 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >O3     is Constrained at      0.520 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F025   is Constrained at      0.473 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F10    is Constrained at      0.480 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F11    is Constrained at      0.480 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F12    is Constrained at      0.480 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F19    is Constrained at      0.473 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F20    is Constrained at      0.473 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F21    is Constrained at      0.473 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F23    is Constrained at      0.473 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F24    is Constrained at      0.473 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F25    is Constrained at      0.473 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F26    is Constrained at      0.473 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F27    is Constrained at      0.473 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F33    is Constrained at      0.480 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F34    is Constrained at      0.480 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F35    is Constrained at      0.480 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F36    is Constrained at      0.480 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F37    is Constrained at      0.480 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F38    is Constrained at      0.480 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of <O1     is Constrained at      0.473 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <O4     is Constrained at      0.480 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C22    is Constrained at      0.527 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C23    is Constrained at      0.527 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C24    is Constrained at      0.527 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C25    is Constrained at      0.520 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C26    is Constrained at      0.520 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C27    is Constrained at      0.520 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C28    is Constrained at      0.520 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C29    is Constrained at      0.473 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C30    is Constrained at      0.473 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C32    is Constrained at      0.473 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C35    is Constrained at      0.480 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C36    is Constrained at      0.480 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C37    is Constrained at      0.480 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C38    is Constrained at      0.480 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Cl1    is Constrained at      0.350 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Cl2    is Constrained at      0.350 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C900   is Constrained at      0.350 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H90A   is Constrained at      0.350 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H90B   is Constrained at      0.350 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Cl3    is Constrained at      0.150 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Cl4    is Constrained at      0.150 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C901   is Constrained at      0.150 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H90C   is Constrained at      0.150 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H90D   is Constrained at      0.150 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =         47 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =        100 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   1.75) in Resd. #          3 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.75) in Resd. #          4 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....          1 Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         10 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....        123 Note
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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
  17 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  87 **ALERT level G** = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  22 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
  79 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.
```

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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.

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

Datablock I - ellipsoid plot