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: 1

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= 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**
            Crystal system given = monoclinic
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.

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PLAT234_ALERT_4_C Large Hirshfeld Difference F17    -- C28    ..      0.17 Ang.
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
PLAT301_ALERT_3_G Main Residue  Disorder ............ Percentage =        47 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ............ Percentage =       100 Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       1 Note
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
  20 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
  12 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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It is advisable to 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 purpose of your study may justify the reported deviations and the more serious of these should normally 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.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 20/08/2014; check.def file version of 18/08/2014

NOMOVE FORCED

Prob = 50
Temp = 123

3 Y

PLATON-Sep 23 15:14:20 2014 - (100912)

Z -158 1   C 1 2/c 1   R = 0.05   RES=   0   -62 X