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 = 0.0153 A         Wavelength=1.54178

Cell:          a=16.7510(5)       b=17.2703(7)     c=18.8355(6)
               alpha=109.136(3)   beta=97.750(3)   gamma=108.799(3)
Temperature:   123 K

                Calculated                 Reported
Volume          4693.8(3)                  4693.8(3)
Space group     P -1                       P -1
Hall group      -P 1                       -P 1
Moiety formula  2(C16 Al F36 O4), 2(C40    2(C40 H60 Cu Mo4 P12),
                H60 Cu Mo4 P12), 5(C7 H8)  2(Al C16 F36 O4), 5(C7 H8)
Sum formula     C147 H160 Al2 Cu2 F72 Mo8  C147 H160 Al2 Cu2 F72 Mo8
                O8 P24                     O8 P24
Mr              5114.62                    5114.58
Dx,g cm-3       1.809                      1.809
Z               1                          1
Mu (mm-1)       7.604                      7.604
F000            2534.0                     2534.0
F000'           2545.21
h,k,lmax        21,21,23                   20,21,23
Nref            19458                      18870
Tmin,Tmax       0.453,0.566                0.759,1.000
Tmin'           0.283

Correction method= # Reported T Limits: Tmin=0.759 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.970          Theta(max)= 75.433

R(reflections)= 0.0665( 16507)    wR2(reflections)= 0.1867( 18870)

S = 1.053                   Npar= 1261
```

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

```
PLAT220_ALERT_2_B Large Non-Solvent  F     Ueq(max)/Ueq(min) Range       10.0 Ratio
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT230_ALERT_2_B Hirshfeld Test Diff for    F8     --  C44     ..         9.0 su
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT230_ALERT_2_B Hirshfeld Test Diff for    F18    --  C48     ..        18.5 su
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C41    --  C42     ..         9.2 su
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C45    --  C47     ..         8.6 su
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT241_ALERT_2_B High      Ueq as Compared to Neighbors for .....        C44 Check
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. C44 is part of a CF3 group.

```
PLAT242_ALERT_2_B Low       Ueq as Compared to Neighbors for .....        C41 Check
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. C41 is a tertiary atom of a tert-butyl group.

```
PLAT250_ALERT_2_B Large U3/U1 Ratio for Average U(i,j) Tensor ....        5.1 Note
PLAT332_ALERT_2_B Large Phenyl C-C Range           C64    -C69            0.28 Ang.
```

Author Response: This is a free toluene molecule in the unit cell.

```
PLAT362_ALERT_2_B Short   C(sp3)-C(sp2) Bond  C57    -   C63    ..        1.31 Ang.
```

Alert level C

```
PLAT213_ALERT_2_C Atom F11             has ADP max/min Ratio .....         3.2 prolat
PLAT213_ALERT_2_C Atom F50A            has ADP max/min Ratio .....         3.2 prolat
PLAT213_ALERT_2_C Atom F51A            has ADP max/min Ratio .....         3.1 prolat
PLAT213_ALERT_2_C Atom F51C            has ADP max/min Ratio .....         3.1 prolat
PLAT213_ALERT_2_C Atom F54C            has ADP max/min Ratio .....         4.0 prolat
PLAT213_ALERT_2_C Atom F55A            has ADP max/min Ratio .....         4.0 prolat
PLAT213_ALERT_2_C Atom F55C            has ADP max/min Ratio .....         3.1 oblate
PLAT213_ALERT_2_C Atom F56A            has ADP max/min Ratio .....         3.3 prolat
PLAT213_ALERT_2_C Atom F56C            has ADP max/min Ratio .....         3.3 prolat
PLAT213_ALERT_2_C Atom C44             has ADP max/min Ratio .....         3.7 prolat
PLAT213_ALERT_2_C Atom C14             has ADP max/min Ratio .....         3.1 prolat
PLAT213_ALERT_2_C Atom C18             has ADP max/min Ratio .....         3.7 prolat
PLAT213_ALERT_2_C Atom C19             has ADP max/min Ratio .....         3.3 prolat
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range         4.8 Ratio
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range         5.4 Ratio
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT222_ALERT_3_C Large Non-Solvent  H     Uiso(max)/Uiso(min) ...         4.2 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F1     --  C42     ..         6.8 su
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F4     --  C43     ..         6.8 su
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F11    --  C46     ..         5.1 su
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT234_ALERT_4_C Large Hirshfeld Difference F3     --  C42     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F6     --  C43     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F13    --  C47     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F14    --  C47     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F16    --  C48     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F50C   --  C50     ..       0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F51A   --  C51     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F51B   --  C51     ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F51C   --  C51     ..       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F52C   --  C52     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F54A   --  C54     ..       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F55B   --  C55     ..       0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F55C   --  C55     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F56B   --  C56     ..       0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C41    --  C44     ..       0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C45    --  C48     ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C53    --  C56     ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C13    --  C14     ..       0.19 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....         O1 Check
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. C44 is part of a CF3 group.

```
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....         O2 Check
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. C44 is part of a CF3 group.

```
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....         O3 Check
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. C44 is part of a CF3 group.

```
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C48 Check
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. C44 is part of a CF3 group.

```
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        Al1 Check
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. C41 is a tertiary atom of a tert-butyl group.

```
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C45 Check
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. C41 is a tertiary atom of a tert-butyl group.

```
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C49 Check
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. C41 is a tertiary atom of a tert-butyl group.

```
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C53 Check
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. C41 is a tertiary atom of a tert-butyl group.

```
PLAT243_ALERT_4_C High  ’Solvent’ Ueq as Compared to Neighbors of         C57 Check
PLAT243_ALERT_4_C High  ’Solvent’ Ueq as Compared to Neighbors of         C59 Check
PLAT243_ALERT_4_C High  ’Solvent’ Ueq as Compared to Neighbors of         C65 Check
PLAT243_ALERT_4_C High  ’Solvent’ Ueq as Compared to Neighbors of         C69 Check
PLAT244_ALERT_4_C Low   ’Solvent’ Ueq as Compared to Neighbors of         C58 Check
PLAT244_ALERT_4_C Low   ’Solvent’ Ueq as Compared to Neighbors of         C61 Check
PLAT244_ALERT_4_C Low   ’Solvent’ Ueq as Compared to Neighbors of         C64 Check
PLAT244_ALERT_4_C Low   ’Solvent’ Ueq as Compared to Neighbors of         C67 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0153 Ang.
PLAT368_ALERT_2_C Short  C(sp2)-C(sp2) Bond  C66    -   C67    ...       1.20 Ang.
PLAT368_ALERT_2_C Short  C(sp2)-C(sp2) Bond  C67    -   C68    ...       1.22 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H62    ..  H93     ..       2.02 Ang.
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         54 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         13 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.11 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      17.28 Why ?
PLAT154_ALERT_1_G The su’s on the Cell Angles are Equal ..........    0.00300 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         14 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records          2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          7 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          5 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F50A   --  C50     ..        6.0 su
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F52B   --  C52     ..        8.9 su
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F54B   --  C54     ..        6.7 su
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F55A   --  C55     ..        5.9 su
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F56A   --  C56     ..        8.8 su
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C49    --  C51     ..        5.9 su
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C49    --  C52     ..        7.2 su
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. The terminal fluorine atoms are strongly affected by this.

```
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo2    --  P6      ..        5.5 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo3    --  P9      ..        5.6 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo3    --  P12     ..        6.0 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo4    --  P8      ..        6.3 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo4    --  P10     ..        5.3 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Mo4    --  P11     ..        5.7 su
PLAT242_ALERT_2_G Low       Ueq as Compared to Neighbors for .....        C42 Check
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. C41 is a tertiary atom of a tert-butyl group.

```
PLAT242_ALERT_2_G Low       Ueq as Compared to Neighbors for .....        C46 Check
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. C41 is a tertiary atom of a tert-butyl group.

```
PLAT242_ALERT_2_G Low       Ueq as Compared to Neighbors for .....        C47 Check
```

Author Response: The weakly coordinating aluminate anion shows heavy disorder and thermal motion. C41 is a tertiary atom of a tert-butyl group.

```
PLAT300_ALERT_4_G Atom Site Occupancy of >F50A   is Constrained at      0.610 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F50B   is Constrained at      0.610 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F50C   is Constrained at      0.610 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F51A   is Constrained at      0.610 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F51B   is Constrained at      0.610 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F51C   is Constrained at      0.610 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F52A   is Constrained at      0.610 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F52B   is Constrained at      0.610 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F52C   is Constrained at      0.610 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F54A   is Constrained at      0.570 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F54B   is Constrained at      0.570 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F54C   is Constrained at      0.570 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F55A   is Constrained at      0.570 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F55B   is Constrained at      0.570 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F55C   is Constrained at      0.570 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F56A   is Constrained at      0.570 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F56B   is Constrained at      0.570 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >F56C   is Constrained at      0.570 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F80A   is Constrained at      0.390 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F80B   is Constrained at      0.390 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F80C   is Constrained at      0.390 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F81A   is Constrained at      0.390 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F81B   is Constrained at      0.390 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F81C   is Constrained at      0.390 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F82A   is Constrained at      0.390 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F82B   is Constrained at      0.390 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F82C   is Constrained at      0.390 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F83A   is Constrained at      0.430 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F83B   is Constrained at      0.430 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F83C   is Constrained at      0.430 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F84A   is Constrained at      0.430 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F84B   is Constrained at      0.430 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F84C   is Constrained at      0.430 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F85A   is Constrained at      0.430 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F85B   is Constrained at      0.430 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <F85C   is Constrained at      0.430 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C50    is Constrained at      0.610 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C51    is Constrained at      0.610 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C52    is Constrained at      0.610 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C54    is Constrained at      0.570 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C55    is Constrained at      0.570 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C56    is Constrained at      0.570 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C80    is Constrained at      0.390 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C81    is Constrained at      0.390 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C82    is Constrained at      0.390 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C83    is Constrained at      0.430 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C84    is Constrained at      0.430 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C85    is Constrained at      0.430 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C90    is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C91    is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C92    is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C93    is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C94    is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C95    is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C96    is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H90    is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H91    is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H92    is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H93    is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H94    is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H96A   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H96B   is Constrained at      0.500 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of *H96C   is Constrained at      0.500 Check
PLAT301_ALERT_3_G Main Residue  Disorder ............ Percentage =         21 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ............ Percentage =         20 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   7.50) in Resd. #          5 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C6 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C7 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C8 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C9 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C10 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C16 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C17 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C18 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C19 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C20 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C26 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C27 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C28 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C29 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C30 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C36 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C37 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C38 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C39 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C40 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C63 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C70 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F2     ..  F56C    ..       2.68 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F4     ..  F56C    ..       2.79 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F11    ..  F50C    ..       2.72 Ang.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         15 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
              C40 H60 Cu Mo4 P12
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............         241 Note
```

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   0 ALERT level A = Most likely a serious problem - resolve or explain
  10 ALERT level B = A potentially serious problem, consider carefully
  57 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 122 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  62 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
 121 ALERT type 4 Improvement, methodology, query or suggestion
   0 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