checkCIF/PLATON report

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: sw257B

Bond precision: C-C = 0.0122 A   Wavelength=1.54178

Cell: a=17.9349(5)   b=17.9349(5)   c=20.9310(7)
                 alpha=90   beta=90   gamma=120
Temperature: 100 K

	Calculated	Reported
Volume	5830.7(3)	5830.7(3)
Space group	P -3	P -3
Hall group	-P 3	-P 3
Moiety formula	C16 Al F36 O4, C21 H15 Cu Mo3 O6 P9	C16 Al F36 O4, C21 H15 Cu Mo3 O6 P9
Sum formula	C37 H15 Al Cu F36 Mo3 O10 P9	C37 H15 Al Cu F36 Mo3 O10 P9
Mr	1960.57	1960.57
Dx,g cm-3	2.233	2.233
Z	4	4
Mu (mm-1)	9.653	9.653
F000	3776.0	3776.0
F000'	3793.80	
h,k,lmax	21,21,24	21,20,24
Nref	6628	6568
Tmin,Tmax	0.536,0.616	0.343,0.666
Tmin'	0.122	

Correction method= ANALYTICAL

Data completeness= 0.991   Theta(max)= 65.070

R(reflections)= 0.0458(5918)   wR2(reflections)= 0.1187(6568)

S = 1.032   Npar= 604

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 A
```
PLAT241_ALERT_2_A Check High     Ueq as Compared to Neighbors for     F4
PLAT241_ALERT_2_A Check High     Ueq as Compared to Neighbors for     F7
PLAT241_ALERT_2_A Check High     Ueq as Compared to Neighbors for     F12
PLAT241_ALERT_2_A Check High     Ueq as Compared to Neighbors for     O7
```

```
PLAT242_ALERT_2_A Check Low       Ueq as Compared to Neighbors for      Al2
PLAT242_ALERT_2_A Check Low       Ueq as Compared to Neighbors for      C21
```

🟠 **Alert level B**
```
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for       F5
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for       F9
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for       O8
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for      C16A
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for      C18B
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for      C22
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for      C23
```

🟡 **Alert level C**
```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
            Calculated sin(theta_max)/wavelength =     0.5882
PLAT213_ALERT_2_C Atom F12              has ADP max/min Ratio .....      3.50 prola
PLAT213_ALERT_2_C Atom C20A             has ADP max/min Ratio .....      3.90 prola
PLAT213_ALERT_2_C Atom C20B             has ADP max/min Ratio .....      3.10 prola
PLAT213_ALERT_2_C Atom O8               has ADP max/min Ratio .....      3.30 prola
PLAT213_ALERT_2_C Atom O3               has ADP max/min Ratio .....      3.10 prola
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       F3
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       F6
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       F8
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       P6
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for      C11
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for      Al1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for      C17
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for      C18A
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for      C19A
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for      C19B
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for      C24
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for      C25
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for      C26
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for      Mo2
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....      2.10
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds (x 1000) Ang ..      12
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond C10    -   C11    ...      1.55 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact  F14    ..  O3       ..      2.83 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Al2    --  O7       ..      0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F15    --  C22      ..      0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O7     --  C21      ..      0.19 Ang.
```

⚪ **Alert level G**
```
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      10.67
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................      6.00 Perc.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......      105
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.       P3
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.       P6
```

```
   6 ALERT level A = In general: serious problem
   7 ALERT level B = Potentially serious problem
  27 ALERT level C = Check and explain
   5 ALERT level G = General alerts; check

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
```

```
36 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
 5 ALERT type 4 Improvement, methodology, query or suggestion
 0 ALERT type 5 Informative message, check
```

PLATON version of 13/08/2009; check.def file version of 12/08/2009

Datablock sw257B - ellipsoid plot