checkCIF/PLATON report

No syntax errors found.   **CIF dictionary**   **Interpreting this report**

Datablock: sw232

```
Bond precision:   C-C = 0.0142 A            Wavelength=1.54178

Cell:           a=14.6968(4)     b=17.9465(5)        c=29.5927(10)
                alpha=90         beta=114.481(3)     gamma=90
Temperature:    100 K
```

	Calculated	Reported
Volume	7103.6(4)	7103.6(4)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C48 H36 Cu2 Mo4 N4 O8 P4, 2(B F4)	C48 H36 Cu2 Mo4 N4 O8 P4, 2(B F4)
Sum formula	C48 H36 B2 Cu2 F8 Mo4 N4 O8 P4	C48 H36 B2 Cu2 F8 Mo4 N4 O8 P4
Mr	1605.17	1605.17
Dx,g cm-3	1.501	1.501
Z	4	4
Mu (mm-1)	7.680	7.680
F000	3136.0	3136.0
F000'	3131.64	
h,k,lmax	17,21,35	17,21,34
Nref	12661	12364
Tmin,Tmax	0.079,0.200	0.096,0.310
Tmin'	0.020	

```
Correction method= GAUSSIAN

Data completeness= 0.977          Theta(max)= 66.890

R(reflections)= 0.0595( 10070)    wR2(reflections)= 0.1689( 12364)

S = 1.073                Npar= 721
```

```
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

```
PLAT241_ALERT_2_B Check High    Ueq as Compared to Neighbors for        C35
PLAT242_ALERT_2_B Check Low     Ueq as Compared to Neighbors for         N2
PLAT242_ALERT_2_B Check Low     Ueq as Compared to Neighbors for        C34
```

```
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......    0.98
PLAT220_ALERT_2_C Large Non-Solvent    C    Ueq(max)/Ueq(min) ...    3.16 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O3    -- C3    ..    5.09 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C34   -- C35   ..    6.26 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Mo2   -- C3    ..    5.43 su
PLAT241_ALERT_2_C Check High    Ueq as Compared to Neighbors for    C23
PLAT241_ALERT_2_C Check High    Ueq as Compared to Neighbors for    C27
PLAT241_ALERT_2_C Check High    Ueq as Compared to Neighbors for    C36
PLAT241_ALERT_2_C Check High    Ueq as Compared to Neighbors for    C37
PLAT242_ALERT_2_C Check Low     Ueq as Compared to Neighbors for    Mo3
PLAT242_ALERT_2_C Check Low     Ueq as Compared to Neighbors for    Mo4
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds (x 1000) Ang ..    14
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of    B1
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of    B2
```

● **Alert level G**

```
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large..    0.10
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.    17.17
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......    114
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure    !
```

```
  0 ALERT level A = In general: serious problem
  3 ALERT level B = Potentially serious problem
 14 ALERT level C = Check and explain
  4 ALERT level G = General alerts; check

  0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 15 ALERT type 2 Indicator that the structure model may be wrong or deficient
  3 ALERT type 3 Indicator that the structure quality may be low
  3 ALERT type 4 Improvement, methodology, query or suggestion
  0 ALERT type 5 Informative message, check
```

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

NOMOVE FORCED

Prob = 50
Temp = 100

O Y

PLATON-Nov 17 17:02:13 2009 - (130809)

Z -146   sw232   P 21/c   R = 0.06   RES=   0   -90 X