

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: sw239B

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Bond precision:    C-C = 0.0095 A

Wavelength=1.54178

Cell:                a=11.4693(5)                b=12.0694(4)                c=14.7956(6)  
                      alpha=69.285(3)            beta=68.390(4)            gamma=88.436(3)  
Temperature:        123 K

	Calculated	Reported
Volume	1768.53(14)	1768.53(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C26 H20 Cu Mo2 N2 O4 P2, C H2 Cl2, B F4	C26 H20 Cu Mo2 N2 O4 P2, C H2 Cl2, B F4
Sum formula	C27 H22 B Cl2 Cu F4 Mo2 N2 O4 P2	C27 H22 B Cl2 Cu F4 Mo2 N2 O4 P2
Mr	913.55	913.55
Dx,g cm-3	1.715	1.715
Z	2	2
Mu (mm-1)	9.154	9.154
F000	896.0	896.0
F000'	896.50	
h,k,lmax	13,14,18	13,14,18
Nref	6701	6632
Tmin,Tmax	0.106,0.178	0.074,0.316
Tmin'	0.009	

Correction method= ANALYTICAL

Data completeness= 0.990

Theta(max)= 70.060

R(reflections)= 0.0517( 6091)

wR2(reflections)= 0.1512( 6632)

S = 1.043

Npar= 406

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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.

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### Alert level C

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C17	--	C18	..	5.03 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo2	--	C14	..	6.20 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1	--	P1	..	6.24 su
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds (x 1000)	Ang	..		9

PLAT431_ALERT_2_C	Short Inter HL..A Contact C11 .. O3 ..	3.11 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C17 -- C20 ..	0.16 Ang.
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of C1S	
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of B1	

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### ● Alert level G

PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large..	0.10
PLAT605_ALERT_4_G	Structure Contains Solvent Accessible VOIDS of .	224.00 A**3
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	2

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 5 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 1 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

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## 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.

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

