

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: sw120b

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Bond precision:    C-C = 0.0075 A

Wavelength=1.54178

Cell:                a=13.1617(3)                b=14.1284(3)                c=17.5214(4)  
                      alpha=102.262(2)        beta=102.025(2)        gamma=90.494(2)  
Temperature:    123 K

	Calculated	Reported
Volume	3109.21(13)	3109.21(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C108 H82 Cu4 Mo4 N8 O8 P6, 4(B F4), 5(C H2 Cl2)	C108 H82 Cu4 Mo4 N8 O8 P6, 4(B F4), 5(C H2 Cl2)
Sum formula	C113 H92 B4 Cl10 Cu4 F16 Mo4 N8 O8 P6	C113 H92 B4 Cl10 Cu4 F16 Mo4 N8 O8 P6
Mr	3215.47	3215.47
Dx,g cm-3	1.717	1.717
Z	1	1
Mu (mm-1)	7.337	7.337
F000	1598.0	1598.0
F000'	1599.06	
h,k,lmax	15,16,20	15,16,20
Nref	9887	9733
Tmin,Tmax	0.459,0.616	0.515,0.704
Tmin'	0.159	

Correction method= MULTI-SCAN

Data completeness= 0.984

Theta(max)= 62.380

R(reflections)= 0.0430( 8472)

wR2(reflections)= 0.1232( 9733)

S = 1.038

Npar= 849

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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 B

THETM01\_ALERT\_3\_B The value of sine(theta\_max)/wavelength is less than 0.575

Calculated sin(theta\_max)/wavelength = 0.5747

PLAT432\_ALERT\_2\_B Short Inter X...Y Contact C33 .. F2B .. 2.78 Ang.



### Alert level C

PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo1	--	C25	..	5.46	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo2	--	C27	..	5.55	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1	--	P1	..	9.12	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1	--	P2	..	5.95	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu2	--	P1	..	6.16	su
PLAT371_ALERT_2_C	Long C(sp2)-C(sp1) Bond	C101	-	C102	...	1.43	Ang.
PLAT371_ALERT_2_C	Long C(sp2)-C(sp1) Bond	C201	-	C202	...	1.44	Ang.
PLAT432_ALERT_2_C	Short Inter X...Y Contact	C29	..	F2B	..	2.89	Ang.
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of						C1S
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						C2S
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of						C3S



### Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	6.94
PLAT301_ALERT_3_G	Note: Main Residue Disorder .....	3.00 Perc.
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints .....	176
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal (x 10000)	200 Deg.
PLAT302_ALERT_4_G	Note: Anion/Solvent Disorder .....	24.00 Perc.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	6

- 0 **ALERT level A** = In general: serious problem  
 2 **ALERT level B** = Potentially serious problem  
 12 **ALERT level C** = Check and explain  
 6 **ALERT level G** = General alerts; check
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 10 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  
 6 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.

