

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

**Datablock: sw247**

---

Bond precision:    C-C = 0.0021 Å

Wavelength=1.54178

Cell:                    a=8.3283(18)  
                          alpha=90

                          b=13.166(3)  
                          beta=90

                          c=12.755(3)  
                          gamma=90

Temperature:            100 K

	Calculated	Reported
Volume	1398.6(5)	1398.6(5)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	C12 H15 Cr O2 P3	C12 H15 Cr O2 P3
Sum formula	C12 H15 Cr O2 P3	C12 H15 Cr O2 P3
Mr	336.15	336.15
Dx, g cm <sup>-3</sup>	1.596	1.596
Z	4	4
Mu (mm <sup>-1</sup> )	9.906	9.906
F000	688.0	688.0
F000'	692.25	
h,k,lmax	9,15,15	9,15,15
Nref	1297	1285
Tmin,Tmax	0.044,0.591	0.089,0.597
Tmin'	0.003	

Correction method= ANALYTICAL

Data completeness= 0.991

Theta(max)= 66.840

R(reflections)= 0.0248( 1219)

wR2(reflections)= 0.0665( 1285)

S = 1.067

Npar= 97

---

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

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	O1	--	C7	..	8.04	su
PLAT232_ALERT_2_B	Hirshfeld Test Diff (M-X)	Cr1	--	C7	..	11.73	su

---



## Alert level C

PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cr1	--	P2	..	6.59	su
-------------------	---------------------------	-----	----	----	----	------	----



---

**Alert level G**

PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	2
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P1
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P2
PLAT380_ALERT_4_G	Check Incorrectly? Oriented X(sp2)-Methyl Moiety	C4

---

0 **ALERT level A** = In general: serious problem

2 **ALERT level B** = Potentially serious problem

1 **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

3 ALERT type 2 Indicator that the structure model may be wrong or deficient

0 ALERT type 3 Indicator that the structure quality may be low

4 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 29/06/2010; check.def file version of 26/06/2010

