

# checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

## Datablock: ds\_01t\_compound\_2

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Bond precision: C-C = 0.0076 Å

Wavelength=0.71073

Cell: a=11.1169(3) b=13.2635(4) c=14.7574(4)  
alpha=89.127(2) beta=84.693(2) gamma=87.350(2)  
Temperature: 100 K

	Calculated	Reported
Volume	2164.19(11)	2164.19(11)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C22 H34 Cl N2 P	C22 H34 Cl N2 P
Sum formula	C22 H34 Cl N2 P	C22 H34 Cl N2 P
Mr	392.93	392.93
Dx,g cm <sup>-3</sup>	1.206	1.206
Z	4	4
Mu (mm <sup>-1</sup> )	0.259	0.259
F000	848.0	848.0
F000'	849.22	
h,k,lmax	13,15,17	13,15,17
Nref	7644	7571
Tmin,Tmax	0.969,0.992	
Tmin'	0.950	

Correction method= Not given

Data completeness= 0.990

Theta(max)= 25.030

R(reflections)= 0.0790( 6181)

wR2(reflections)= 0.2122( 7571)

S = 1.158

Npar= 474

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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

PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 8  
PLAT480\_ALERT\_4\_C Long H...A H-Bond Reported H19C .. CL1' .. 2.86 Ang.

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### Alert level G

PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large. 11.28

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

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