

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

**Datablock: phw1301**

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Bond precision:    C-C = 0.0030 Å

Wavelength=0.71070

Cell:                    a=11.6014(5)            b=9.7929(4)            c=29.2781(12)  
                          alpha=90            beta=90.850(4)            gamma=90  
Temperature:            110 K

	Calculated	Reported
Volume	3326.0(2)	3326.0(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C33 H42 N6, C2 H6 O	C33 H42 N6, C2 H6 O
Sum formula	C35 H48 N6 O	C35 H48 N6 O
Mr	568.79	568.79
Dx, g cm <sup>-3</sup>	1.136	1.136
Z	4	4
Mu (mm <sup>-1</sup> )	0.070	0.070
F000	1232.0	1232.0
F000'	1232.40	
h,k,lmax	15,12,38	15,12,38
Nref	8019	6771
Tmin,Tmax	0.986,0.997	0.987,0.997
Tmin'	0.984	

Correction method= ANALYTICAL

Data completeness= 0.844

Theta(max)= 28.000

R(reflections)= 0.0598( 4850)

wR2(reflections)= 0.1414( 6771)

S = 1.049

Npar= 410

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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

PLAT220\_ALERT\_2\_C Large Non-Solvent      C      Ueq(max)/Ueq(min) ...      3.2 Ratio

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## Alert level G

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite      5  
PLAT005\_ALERT\_5\_G No \_iucr\_refine\_instructions\_details in the CIF      ? Do !

PLAT128_ALERT_4_G	Note: Alternate Setting of Space-group P21/c	P21/n
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	C34A
PLAT302_ALERT_4_G	Note: Anion/Solvent Disorder .....	67 %
PLAT380_ALERT_4_G	Check Incorrectly? Oriented X(sp2)-Methyl Moiety	C24
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints .....	4

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0	<b>ALERT level A</b>	= Most likely a serious problem - resolve or explain
0	<b>ALERT level B</b>	= A potentially serious problem, consider carefully
1	<b>ALERT level C</b>	= Check. Ensure it is not caused by an omission or oversight
7	<b>ALERT level G</b>	= General information/check it is not something unexpected

  

0	ALERT type 1	CIF construction/syntax error, inconsistent or missing data
2	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
4	ALERT type 4	Improvement, methodology, query or suggestion
1	ALERT type 5	Informative message, check

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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

#### 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.

