

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

**Datablock: phw1118**

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Bond precision:    C-C = 0.0045 Å

Wavelength=0.71070

Cell:                    a=14.2781(7)  
                          alpha=90

b=14.2781(7)  
beta=90

c=7.8801(4)  
gamma=120

Temperature:          110 K

	Calculated	Reported
Volume	1391.24(18)	1391.26(12)
Space group	P 3 1 c	P 3 1 c
Hall group	P 3 -2c	P 3 -2c
Moiety formula	C30 H39 N3 O3	C30 H39 N3 O3
Sum formula	C30 H39 N3 O3	C30 H39 N3 O3
Mr	489.64	489.64
Dx, g cm <sup>-3</sup>	1.169	1.169
Z	2	2
Mu (mm <sup>-1</sup> )	0.076	0.076
F000	528.0	528.0
F000'	528.21	
h,k,lmax	21,21,11	18,20,11
Nref	1644[ 3270]	2325
Tmin,Tmax	0.985,0.989	0.993,0.996
Tmin'	0.976	

Correction method= ANALYTICAL

Data completeness= 1.41/0.71

Theta(max)= 32.160

R(reflections)= 0.0622( 1942)

wR2(reflections)= 0.1929( 2325)

S = 1.088

Npar= 118

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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

STRVA01\_ALERT\_4\_C                    Flack parameter is too small

From the CIF: \_refine\_ls\_abs\_structure\_Flack    -1.000

From the CIF: \_refine\_ls\_abs\_structure\_Flack\_su    2.000

PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.0045 Ang

PLAT790\_ALERT\_4\_C Centre of Gravity not Within Unit Cell: Resd. # 1

C30 H39 N3 O3

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● **Alert level G**

REFLT03\_ALERT\_1\_G ALERT: Expected hkl max differ from CIF values  
From the CIF: \_diffrn\_reflns\_theta\_max 32.16  
From the CIF: \_reflns\_number\_total 2325  
From the CIF: \_diffrn\_reflns\_limit\_max hkl 8. 19. 9.  
From the CIF: \_diffrn\_reflns\_limit\_min hkl -18. -20. -11.  
TEST1: Expected hkl limits for theta max  
Calculated maximum hkl 21. 21. 11.  
Calculated minimum hkl -21. -21. -11.  
REFLT03\_ALERT\_4\_G ALERT: MoKa measured Friedel data cannot be used to  
determine absolute structure in a light-atom  
study EXCEPT under VERY special conditions.  
It is preferred that Friedel data is merged in such cases.  
From the CIF: \_diffrn\_reflns\_theta\_max 32.16  
From the CIF: \_reflns\_number\_total 2325  
Count of symmetry unique reflns 1644  
Completeness (\_total/calc) 141.42%  
TEST3: Check Friedels for noncentro structure  
Estimate of Friedel pairs measured 681  
Fraction of Friedel pairs measured 0.414  
Are heavy atom types Z>Si present no  
PLAT005\_ALERT\_5\_G No \_iucr\_refine\_instructions\_details in CIF .... ?  
PLAT032\_ALERT\_4\_G Std. Uncertainty on Flack Parameter Value High . 2.000  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large. 0.12  
PLAT152\_ALERT\_1\_G The Supplied and Calc. Volume s.u. Differ by ... 6 Units  
PLAT950\_ALERT\_5\_G Reported and Calculated Hmax Values Differ by .. 3

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

2 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  
4 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

