

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: 1

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Bond precision:	C-C = 0.0032 Å	Wavelength=0.71073	
Cell:	a=19.398(3)	b=10.0574(15)	c=21.725(4)
	alpha=90	beta=107.917(6)	gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	4032.9(11)	4032.9(11)	
Space group	C 2/c	C 2/c	
Hall group	-C 2yc	-C 2yc	
Moiety formula	C26 H18 N2	?	
Sum formula	C26 H18 N2	C26 H18 N2	
Mr	358.42	358.42	
Dx,g cm-3	1.181	1.181	
Z	8	8	
Mu (mm-1)	0.069	0.069	
F000	1504.0	1504.0	
F000'	1504.52		
h,k,lmax	22,11,25	22,11,25	
Nref	3533	3505	
Tmin,Tmax	0.982,0.985		
Tmin'	0.982		

Correction method= Not given

Data completeness= 0.992      Theta(max)= 24.996

R(reflections)= 0.0456( 1704)      wR2(reflections)= 0.0918( 3505)

S = 0.846      Npar= 253

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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

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..	49%	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C21	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	41.107	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.254	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	5.268	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.076	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	5	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.595	23	Report

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### ● Alert level G

PLAT230_ALERT_2_G	Hirshfeld Test Diff for C9 --C11 .	7.5	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C14 --C19 .	5.6	s.u.
PLAT371_ALERT_2_G	Long C(sp2)-C(sp1) Bond C14 - C19 .	1.44	Ang.
PLAT371_ALERT_2_G	Long C(sp2)-C(sp1) Bond C20 - C21 .	1.44	Ang.
PLAT793_ALERT_4_G	Model has Chirality at C7 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C8 (Centro SPGR)	R	Verify
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	20	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	2.8	Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....	Please	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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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  
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
11 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
7 ALERT type 2 Indicator that the structure model may be wrong or deficient  
8 ALERT type 3 Indicator that the structure quality may be low  
2 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* or *IUCrData*, 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.

