

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp\_145

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: exp\_145

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Bond precision:	C-C = 0.0040 A	Wavelength=0.71073	
Cell:	a=6.8084 (10)	b=16.270 (2)	c=24.839 (2)
	alpha=90	beta=90	gamma=90
Temperature:	295 K		
	Calculated	Reported	
Volume	2751.5 (6)	2751.5 (6)	
Space group	P b c a	P b c a	
Hall group	-P 2ac 2ab	-P 2ac 2ab	
Moiety formula	C17 H14 N2 O	C17 H14 N2 O	
Sum formula	C17 H14 N2 O	C17 H14 N2 O	
Mr	262.30	262.30	
Dx, g cm <sup>-3</sup>	1.266	1.266	
Z	8	8	
Mu (mm <sup>-1</sup> )	0.080	0.080	
F000	1104.0	1104.0	
F000'	1104.43		
h, k, lmax	9, 23, 36	9, 23, 34	
Nref	4448	3788	
Tmin, Tmax	0.968, 0.980	0.733, 1.000	
Tmin'	0.964		

Correction method= # Reported T Limits: Tmin=0.733 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.852      Theta(max)= 31.190

R(reflections)= 0.0715 ( 1754)	wR2(reflections)=
S = 1.010	0.2466 ( 3788)
Npar= 207	

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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 B**

PLAT031\_ALERT\_4\_B Refined Extinction Parameter Within Range of ... 1.867 Sigma

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#### **Alert level C**

PLAT026\_ALERT\_3\_C Ratio Observed / Unique Reflections (too) Low .. 46% Check  
PLAT905\_ALERT\_3\_C Negative K value in the Analysis of Variance ... -2.057 Report  
PLAT910\_ALERT\_3\_C Missing # of FCF Reflection(s) Below Theta(Min). 8 Note  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 26 Report

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#### **Alert level G**

PLAT012\_ALERT\_1\_G No \_shelx\_res\_checksum Found in CIF ..... Please Check  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.10 Report  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 613 Note  
PLAT913\_ALERT\_3\_G Missing # of Very Strong Reflections in FCF .... 1 Note  
PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 10 Note  
PLAT952\_ALERT\_5\_G Calculated (ThMax) and CIF-Reported Lmax Differ. 2 Units  
PLAT958\_ALERT\_1\_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 2 Units  
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  
1 **ALERT level B** = A potentially serious problem, consider carefully  
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
8 **ALERT level G** = General information/check it is not something unexpected

- 2 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  
5 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.

