

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dg13\_3

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: dg13\_3

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Bond precision:    C-C = 0.0045 Å                      Wavelength=1.54184

Cell:                      a=6.6485(13)              b=16.561(3)              c=9.990(2)  
                                alpha=90                      beta=107.90(3)              gamma=90

Temperature:              173 K

	Calculated	Reported
Volume	1046.7(4)	1046.7(3)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C20 H20 N4, 2(B F4)	?
Sum formula	C20 H20 B2 F8 N4	C20 H20 B2 F8 N4
Mr	490.02	490.02
Dx, g cm <sup>-3</sup>	1.555	1.555
Z	2	2
Mu (mm <sup>-1</sup> )	1.255	1.255
F000	500.0	500.0
F000'	502.08	
h,k,lmax	8,19,12	7,19,12
Nref	1904	1831
Tmin,Tmax	0.798,0.860	0.770,0.864
Tmin'	0.759	

Correction method= # Reported T Limits: Tmin=0.770 Tmax=0.864  
AbsCorr = MULTI-SCAN

Data completeness= 0.962                      Theta(max)= 68.230

R(reflections)= 0.0826( 1405)              wR2(reflections)= 0.2356( 1831)

S = 1.066                      Npar= 154

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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 A

RINTA01\_ALERT\_3\_A The value of Rint is greater than 0.25  
Rint given 0.400  
PLAT020\_ALERT\_3\_A The value of Rint is greater than 0.12 ..... 0.400 Report

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### Alert level C

PLAT029\_ALERT\_3\_C \_diffn\_measured\_fraction\_theta\_full value Low . 0.961 Note  
PLAT250\_ALERT\_2\_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.9 Note  
PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.0045 Ang.  
PLAT906\_ALERT\_3\_C Large K value in the Analysis of Variance ..... 112.561 Check  
PLAT906\_ALERT\_3\_C Large K value in the Analysis of Variance ..... 8.818 Check  
PLAT906\_ALERT\_3\_C Large K value in the Analysis of Variance ..... 2.761 Check  
PLAT906\_ALERT\_3\_C Large K value in the Analysis of Variance ..... 8.740 Check  
PLAT906\_ALERT\_3\_C Large K value in the Analysis of Variance ..... 2.340 Check  
PLAT906\_ALERT\_3\_C Large K value in the Analysis of Variance ..... 2.700 Check  
PLAT906\_ALERT\_3\_C Large K value in the Analysis of Variance ..... 3.526 Check  
PLAT911\_ALERT\_3\_C Missing # FCF Refl Between THmin & STh/L= 0.600 73 Report  
PLAT977\_ALERT\_2\_C Check the Negative Difference Density on H32A -0.32 eA-3

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### Alert level G

PLAT005\_ALERT\_5\_G No Embedded Refinement Details found in the CIF Please Do !  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.13 Report  
PLAT244\_ALERT\_4\_G Low 'Solvent' Ueq as Compared to Neighbors of B11 Check  
PLAT371\_ALERT\_2\_G Long C(sp2)-C(sp1) Bond C13 - C18 .. 1.41 Ang.  
PLAT380\_ALERT\_4\_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C32 Check  
PLAT380\_ALERT\_4\_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C33 Check  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 13 Do !  
C13 -C13 -C18 -N2 51.00 12.00 3.655 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 14 Do !  
C13 -C13 -C18 -N9 -128.00 12.00 3.655 1.555 1.555 1.555  
PLAT899\_ALERT\_4\_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density 3 Note

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
5 ALERT type 2 Indicator that the structure model may be wrong or deficient  
12 ALERT type 3 Indicator that the structure quality may be low  
6 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.

