

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) t

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: t

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Bond precision:    C-C = 0.0041 Å                      Wavelength=0.71073

Cell:                      a=9.29800              b=19.00800              c=15.95600  
                                alpha=90              beta=96.7100              gamma=90  
Temperature:              293 K

	Calculated	Reported
Volume	2800.689	2801
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C35 H30 O5	?
Sum formula	C35 H30 O5	C35 H30 O5
Mr	530.59	530.59
Dx, g cm <sup>-3</sup>	1.258	1.258
Z	4	4
Mu (mm <sup>-1</sup> )	0.083	0.083
F000	1120.0	1120.0
F000'	1120.54	
h,k,lmax	11,22,18	11,22,18
Nref	4930	4904
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.995                      Theta(max)= 24.997

R(reflections)= 0.0751( 4120)              wR2(reflections)= 0.1561( 4904)

S = 1.147                      Npar= 365

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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

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...		Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...		Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...		Please Check
PLAT141_ALERT_4_C	s.u. on a - Axis Small or Missing .....	0.00000	Ang.
PLAT142_ALERT_4_C	s.u. on b - Axis Small or Missing .....	0.00000	Ang.
PLAT143_ALERT_4_C	s.u. on c - Axis Small or Missing .....	0.00000	Ang.
PLAT145_ALERT_4_C	s.u. on beta Small or Missing .....	0.0000	Degree
PLAT151_ALERT_1_C	No s.u. (esd) Given on Volume .....		Please Do !
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00405	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	21.154	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	3.501	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595	26 Report

### ● Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	1	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature .... (K)	293	Check
PLAT793_ALERT_4_G	Model has Chirality at C13 (Centro SPGR)		R Verify
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	66%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	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  
13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
9 **ALERT level G** = General information/check it is not something unexpected

- 7 **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  
7 **ALERT type 3** Indicator that the structure quality may be low  
5 **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.

