

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) f3-b-100k

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: f3-b-100k

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Bond precision:    C-C = 0.0019 A                      Wavelength=0.79990

Cell:              a=9.890(2)              b=12.050(2)              c=12.290(3)  
                    alpha=84.45(3)              beta=88.28(3)              gamma=88.54(3)

Temperature:      100 K

	Calculated	Reported
Volume	1456.8(5)	1456.8(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H36	;C44H36;
Sum formula	C44 H36	C44 H36
Mr	564.73	564.73
Dx,g cm-3	1.287	1.287
Z	2	2
Mu (mm-1)	0.091	0.094
F000	600.0	600.0
F000'	600.31	
h,k,lmax	14,17,18	14,17,16
Nref	10154	7962
Tmin,Tmax	0.994,0.995	
Tmin'	0.991	

Correction method= Not given

Data completeness= 0.784                      Theta(max)= 36.654

R(reflections)= 0.0615( 7513)              wR2(reflections)= 0.1686( 7962)

S = 1.032                                      Npar= 403

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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**

PLAT029\_ALERT\_3\_A \_diffrn\_measured\_fraction\_theta\_full value Low . 0.919 Why?

**Author Response: This is caused by the limited data collection strategy with the synchrotron facility.**

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**Alert level B**

PLAT097\_ALERT\_2\_B Large Reported Max. (Positive) Residual Density 0.70 eA-3

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**Alert level C**

DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75  
The relevant atom site should be identified.

PLAT052\_ALERT\_1\_C Info on Absorption Correction Method Not Given Please Do !  
PLAT410\_ALERT\_2\_C Short Intra H...H Contact H15 ..H26 . 1.90 Ang.  
x,y,z = 1\_555 Check

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.746 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 425 Report

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**Alert level G**

FORMU01\_ALERT\_1\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and \_chemical\_formula\_moiety. This is  
usually due to the moiety formula being in the wrong format.  
Atom count from \_chemical\_formula\_sum: C44 H36  
Atom count from \_chemical\_formula\_moiety:

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
not performed for this radiation type.

PLAT042\_ALERT\_1\_G Calc. and Reported MoietyFormula Strings Differ Please Check  
PLAT092\_ALERT\_4\_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.79990 Ang.  
PLAT154\_ALERT\_1\_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.03 Degree  
PLAT180\_ALERT\_4\_G Check Cell Rounding: # of Values Ending with 0 = 3 Note  
PLAT333\_ALERT\_2\_G Large Aver C6-Ring C-C Dist C2 -C22 . 1.42 Ang.  
PLAT333\_ALERT\_2\_G Large Aver C6-Ring C-C Dist C12 -C17 . 1.42 Ang.  
PLAT793\_ALERT\_4\_G Model has Chirality at C1 (Centro SPGR) S Verify  
PLAT793\_ALERT\_4\_G Model has Chirality at C10 (Centro SPGR) S Verify  
PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 1617 Note  
PLAT913\_ALERT\_3\_G Missing # of Very Strong Reflections in FCF .... 3 Note  
PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 3.4 Low  
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. 17 Info  
PLAT984\_ALERT\_1\_G The C-f'= 0.0033 Deviates from the B&C-Value 0.0043 Check

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

- 9 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  
5 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.

