

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

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Bond precision:	C-C = 0.0048 A	Wavelength=1.54184	
Cell:	a=5.26628(17)	b=12.9714(4)	c=16.6563(5)
	alpha=90	beta=90	gamma=90
Temperature:	123 K		
	Calculated	Reported	
Volume	1137.81(6)	1137.81(6)	
Space group	P 21 21 21	P 21 21 21	
Hall group	P 2ac 2ab	P 2ac 2ab	
Moiety formula	C18 H12	C18 H12	
Sum formula	C18 H12	C18 H12	
Mr	228.28	228.28	
Dx,g cm-3	1.333	1.333	
Z	4	4	
Mu (mm-1)	0.572	0.572	
F000	480.0	480.0	
F000'	481.24		
h,k,lmax	6,16,20	6,16,20	
Nref	2369[ 1403]	2324	
Tmin,Tmax	0.825,0.907	0.956,1.000	
Tmin'	0.795		

Correction method= MULTI-SCAN

Data completeness= 1.66/0.98      Theta(max)= 75.518

R(reflections)= 0.0550( 2039)      wR2(reflections)= 0.1610( 2324)

S = 1.043      Npar= Npar = 163

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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**

DIFMX01\_ALERT\_2\_B The maximum difference density is > 0.1\*ZMAX\*1.00  
  \_refine\_diff\_density\_max given = 0.949  
  Test value = 0.600  
  Crystal system given = orthorhombic  
PLAT094\_ALERT\_2\_B Ratio of Maximum / Minimum Residual Density .... 4.87 Why ?  
PLAT097\_ALERT\_2\_B Large Reported Max. (Positive) Residual Density 0.95 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.  
STRVA01\_ALERT\_4\_C Flack parameter is too small  
  From the CIF: \_refine\_ls\_abs\_structure\_Flack -1.600  
  From the CIF: \_refine\_ls\_abs\_structure\_Flack\_su 1.000  
PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.0048 Ang.  
PLAT410\_ALERT\_2\_C Short Intra H...H Contact H10A .. H11A .. 1.99 Ang.

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🟡 **Alert level G**

PLAT032\_ALERT\_4\_G Std. Uncertainty on Flack Parameter Value High . 1.000 Why ?  
PLAT333\_ALERT\_2\_G Check Large Av C6-Ring C-C Dist. C1 -C6 1.44 Ang.  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 11 Note  
PLAT916\_ALERT\_2\_G Hooft y and Flack x Parameter values differ by . 0.90 Check

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  - 6 ALERT type 2 Indicator that the structure model may be wrong or deficient
  - 1 ALERT type 3 Indicator that the structure quality may be low
  - 3 ALERT type 4 Improvement, methodology, query or suggestion
  - 0 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*, 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.

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**PLATON version of 05/02/2014; check.def file version of 05/02/2014**

