

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2

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: 2

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Bond precision:    C-C = 0.0031 A                      Wavelength=0.71075

Cell:                      a=4.8832(7)              b=7.5868(12)              c=35.478(6)  
                                    alpha=90              beta=90                      gamma=90

Temperature:              93 K

	Calculated	Reported
Volume	1314.4(4)	1314.4(4)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C11 H16 O7	C11 H16 O7
Sum formula	C11 H16 O7	C11 H16 O7
Mr	260.24	260.24
Dx,g cm-3	1.315	1.315
Z	4	4
Mu (mm-1)	0.111	0.111
F000	552.0	552.0
F000'	552.39	
h,k,lmax	5,9,42	5,9,42
Nref	2372[ 1442]	2275
Tmin,Tmax	0.996,0.998	0.543,0.998
Tmin'	0.987	

Correction method= # Reported T Limits: Tmin=0.543 Tmax=0.998  
AbsCorr = MULTI-SCAN

Data completeness= 1.58/0.96                      Theta(max)= 25.300

R(reflections)= 0.0360( 2149)                      wR2(reflections)= 0.0899( 2275)

S = 1.048    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 C**

STRVA01\_ALERT\_4\_C                    Flack parameter is too small  
    From the CIF: `_refine_ls_abs_structure_Flack`    -0.400  
    From the CIF: `_refine_ls_abs_structure_Flack_su`    0.700  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L=    0.600                    13 Report

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**Alert level G**

PLAT032\_ALERT\_4\_G Std. Uncertainty on Flack Parameter Value High .            0.700 Report  
PLAT398\_ALERT\_2\_G Deviating C-O-C    Angle From 120 for O1            108.5 Degree  
PLAT398\_ALERT\_2\_G Deviating C-O-C    Angle From 120 for O4            108.0 Degree  
PLAT791\_ALERT\_4\_G Model has Chirality at C3                    (Chiral SPGR)            S Verify  
PLAT791\_ALERT\_4\_G Model has Chirality at C5                    (Chiral SPGR)            R Verify  
PLAT791\_ALERT\_4\_G Model has Chirality at C8                    (Chiral SPGR)            S Verify  
PLAT882\_ALERT\_1\_G No Datum for `_diffn_refl` `av_unetI/netI` .....            Please Do !  
PLAT909\_ALERT\_3\_G Percentage of I>2sig(I) Data at Theta(Max) Still            84% Note  
PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min).            2 Note  
PLAT916\_ALERT\_2\_G Hooft y and Flack x Parameter Values Differ by .            0.18 Check  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density.            3 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  
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
11 **ALERT level G** = General information/check it is not something unexpected

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

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**PLATON version of 22/12/2019; check.def file version of 13/12/2019**

