

## checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: -Trimethoxybenzaldehyde

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Bond precision:    C-C = 0.0030 Å                      Wavelength=0.71070

Cell:                      a=4.0759(8)              b=7.454(2)              c=31.817(5)  
                                alpha=90              beta=90.813(17)              gamma=90

Temperature:              293 K

	Calculated	Reported
Volume	966.6(4)	966.5(4)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C10 H12 O4	C10 H12 O4
Sum formula	C10 H12 O4	C10 H12 O4
Mr	196.20	196.20
Dx, g cm <sup>-3</sup>	1.348	1.348
Z	4	4
Mu (mm <sup>-1</sup> )	0.104	0.104
F000	416.0	416.0
F000'	416.26	
h, k, lmax	6, 11, 47	6, 11, 46
Nref	3316	2491
Tmin, Tmax	0.991, 0.996	1.000, 1.000
Tmin'	0.988	

Correction method= # Reported T Limits: Tmin=1.000 Tmax=1.000  
AbsCorr = NONE

Data completeness= 0.751                      Theta(max)= 31.912

R(reflections)= 0.0509( 1260)                      wR2(reflections)=  
S = 1.150                      Npar= 127                      wR= 0.0412( 1260)

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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 G**

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293 Check
PLAT728_ALERT_1_G	D-H..A Calc 145.00, Rep 1145.00 Dev...	1000.00 Degree
	C10 -H101 -O3 1_555 1_555 3_746 #	1 Check
PLAT769_ALERT_4_G	CIF Embedded explicitly supplied scattering data	Please Note
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please Check
PLAT882_ALERT_1_G	No Datum for _diffrn_reflms_av_unetI/netI .....	Please Do !

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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  
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
7 **ALERT level G** = General information/check it is not something unexpected

- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
0 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
2 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 28/11/2022; check.def file version of 28/11/2022** \*Error: could not change to directory '-Trimethoxybenzaldehyde', stopped