

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) s

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: s

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Bond precision:    C-C = 0.0067 A

Wavelength=1.54178

Cell:              a=10.9288(3)              b=11.7408(4)              c=15.7438(5)  
                    alpha=84.345(2)              beta=69.749(2)              gamma=66.639(2)  
Temperature:    162 K

	Calculated	Reported
Volume	1738.14(10)	1738.14(10)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C26 H44 O2	C26 H44 O2
Sum formula	C26 H44 O2	C26 H44 O2
Mr	388.61	388.61
Dx,g cm-3	1.114	1.114
Z	3	3
Mu (mm-1)	0.513	0.513
F000	648.0	648.0
F000'	649.63	
h,k,lmax	13,14,18	13,14,18
Nref	12780[ 6390]	12355
Tmin,Tmax	0.782,0.857	0.550,0.753
Tmin'	0.774	

Correction method= # Reported T Limits: Tmin=0.550 Tmax=0.753  
AbsCorr = MULTI-SCAN

Data completeness= 1.93/0.97

Theta(max)= 68.458

R(reflections)= 0.0562( 9786)

wR2(reflections)= 0.1658( 12355)

S = 1.059

Npar= 781

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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**

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ...	2.84	Report
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	0.70	eA-3
PLAT234_ALERT_4_C	Large Hirshfeld Difference O6 --C78	0.16	Ang.
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00675	Ang.
PLAT601_ALERT_2_C	Unit Cell Contains Solvent Accessible VOIDS of .	54	Ang**3

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● **Alert level G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	6	Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002	Degree
PLAT791_ALERT_4_G	Model has Chirality at C2 (Sohnke SpGr)		R Verify
PLAT791_ALERT_4_G	Model has Chirality at C4 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C6 (Sohnke SpGr)		R Verify
PLAT791_ALERT_4_G	Model has Chirality at C7 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C8 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C10 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C11 (Sohnke SpGr)		R Verify
PLAT791_ALERT_4_G	Model has Chirality at C14 (Sohnke SpGr)		R Verify
PLAT791_ALERT_4_G	Model has Chirality at C18 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C21 (Sohnke SpGr)		R Verify
PLAT791_ALERT_4_G	Model has Chirality at C23 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C27 (Sohnke SpGr)		R Verify
PLAT791_ALERT_4_G	Model has Chirality at C29 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C30 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C34 (Sohnke SpGr)		R Verify
PLAT791_ALERT_4_G	Model has Chirality at C36 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C39 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C42 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C49 (Sohnke SpGr)		R Verify
PLAT791_ALERT_4_G	Model has Chirality at C52 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C53 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C58 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C69 (Sohnke SpGr)		S Verify
PLAT791_ALERT_4_G	Model has Chirality at C74 (Sohnke SpGr)		S Verify
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	29	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	9	Check

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

2 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  
1 ALERT type 3 Indicator that the structure quality may be low  
26 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 18/09/2020; check.def file version of 20/08/2020**

