

# 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: Cu1\_a

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Bond precision:	C-C = 0.0113 A	Wavelength=1.54178
Cell:	a=10.5965(5)	b=35.9665(16)      c=25.1721(11)
	alpha=90	beta=92.663(3)      gamma=90
Temperature:	103 K	
	Calculated	Reported
Volume	9583.2(7)	9583.2(7)
Space group	C c	C c
Hall group	C -2yc	C -2yc
Moiety formula	C106 H164 O6	?
Sum formula	C106 H164 O6	C106 H164 O6
Mr	1534.37	1534.36
Dx,g cm-3	1.064	1.063
Z	4	4
Mu (mm-1)	0.478	0.478
F000	3392.0	3392.0
F000'	3400.47	
h,k,lmax	12,43,30	12,43,30
Nref	18201[ 9111]	17547
Tmin,Tmax	0.933,0.944	0.649,0.744
Tmin'	0.922	
Correction method= # Reported T Limits: Tmin=0.649 Tmax=0.744		
AbsCorr = MULTI-SCAN		
Data completeness=	1.93/0.96	Theta(max)= 70.168
R(reflections)=	0.0852( 11531)	wR2(reflections)= 0.2743( 17547)
S =	1.075	Npar= 1272

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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

PLAT340\_ALERT\_3\_B Low Bond Precision on C-C Bonds ..... 0.01129 Ang.

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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.

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25) .....	0.27	Report
PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18) .....	7.16	Note
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	2.50	Report
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	0.69	eA-3
PLAT234_ALERT_4_C	Large Hirshfeld Difference C28_1 --C30_1 .	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C17_2 --C18_2 .	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C16_4 --C17_4 .	0.16	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C16_1		Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C19_1		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C15_1		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C18_1		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C18_2		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C7_4		Check

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## 🟡 Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	70	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	137	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	2	Report
PLAT032_ALERT_4_G	Std. Uncertainty on Flack Parameter Value High .	0.500	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	6	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	9	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	2	Report
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	22%	Note
PLAT411_ALERT_2_G	Short Inter H...H Contact H19B_1 ..H19B_3 .	2.14	Ang.
	x,1-y,1/2+z =	2_565	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H2A_1 ..H10A_1 .	2.12	Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H23_1 ..H30B_1 .	2.08	Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H25_1 ..H31A_1 .	2.00	Ang.
	x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H4_3 ..H8AB_3 .	2.14	Ang.
	x,y,z =	1_555	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	342	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	3718	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

14 **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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

16 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

9 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.

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**PLATON version of 05/12/2020; check.def file version of 05/12/2020**

