

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu\_BUN623F2A\_3\_0m\_a

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: cu\_BUN623F2A\_3\_0m\_a

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Bond precision:    C-C = 0.0057 A                      Wavelength=1.54178

Cell:              a=7.4475(5)              b=7.7239(5)              c=14.5814(10)  
                    alpha=97.298(3)          beta=93.052(3)          gamma=115.003(3)

Temperature:      150 K

	Calculated	Reported
Volume	748.66(9)	748.66(9)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C32 H54 O5	?
Sum formula	C32 H54 O5	C8 H13.50 O1.25
Mr	518.75	129.69
Dx,g cm-3	1.151	1.151
Z	1	4
Mu (mm-1)	0.592	0.592
F000	286.0	286.0
F000'	286.79	
h,k,lmax	9,9,17	9,9,17
Nref	5896[ 2948]	5573
Tmin,Tmax	0.876,0.937	0.706,0.754
Tmin'	0.817	

Correction method= # Reported T Limits: Tmin=0.706 Tmax=0.754  
AbsCorr = MULTI-SCAN

Data completeness= 1.89/0.95                      Theta(max)= 72.096

R(reflections)= 0.0479( 5177)                      wR2(reflections)= 0.1278( 5573)

S = 1.036    Npar= 349

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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**

PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C13	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C18	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C22	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C27	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C14	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C19	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C20	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C24	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C25	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C28	Check
PLAT340_ALERT_3_C	Low	Bond Precision on C-C Bonds	.....	0.00574	Ang.
PLAT412_ALERT_2_C	Short	Intra XH3 .. XHn	H13A ..H21A	.	1.88 Ang.
			x,y,z =	1_555	Check
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & STh/L=	0.600	48	Report
PLAT913_ALERT_3_C	Missing	# of Very Strong Reflections in FCF	....	6	Note

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● **Alert level G**

PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.25	Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.003	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	2	Note
PLAT791_ALERT_4_G	Model has Chirality at C3 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C9 (Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C11 (Sohnke SpGr)	S	Verify
PLAT791_ALERT_4_G	Model has Chirality at C14 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C16 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C19 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C20 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C24 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C25 (Sohnke SpGr)	R	Verify
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	14	Note
PLAT915_ALERT_3_G	No Flack x Check Done: Low Friedel Pair Coverage	91	%
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	4	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  
14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
17 **ALERT level G** = General information/check it is not something unexpected
- 3 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data  
12 **ALERT type 2** Indicator that the structure model may be wrong or deficient  
4 **ALERT type 3** Indicator that the structure quality may be low  
11 **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 08/07/2020; check.def file version of 17/06/2020**

