

# checkCIF/PLATON report

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

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: I

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Bond precision:    C-C = 0.0191 Å                      Wavelength=1.54184

Cell:                      a=63.515(5)              b=63.515(5)              c=63.515(5)  
                                alpha=90              beta=90              gamma=90

Temperature:              225 K

	Calculated	Reported
Volume	256229(61)	256229(61)
Space group	F m -3 m	F m -3 m
Hall group	-F 4 2 3	-F 4 2 3
Moiety formula	C24 H12 Cu O4	C24 H12 Cu O4
Sum formula	C24 H12 Cu O4	C24 H12 Cu O4
Mr	427.89	427.88
Dx, g cm-3	0.266	0.266
Z	96	96
Mu (mm-1)	0.332	0.332
F000	20832.0	20832.0
F000'	20700.71	
h,k,lmax	46,46,46	26,32,45
Nref	2680	2600
Tmin,Tmax	0.926,0.977	0.927,0.977
Tmin'	0.926	

Correction method= MULTI-SCAN

Data completeness= 0.970                      Theta(max)= 34.660

R(reflections)= 0.0727( 1174)              wR2(reflections)= 0.2013( 2600)

S = 0.862                      Npar= 145

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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 A

TYPE025\_ALERT\_1\_A \_cell\_volume not of type numb.

**Author Response: CheckCIF truncates volume if reported as type numb.**

THETM01\_ALERT\_3\_A The value of sine(theta\_max)/wavelength is less than 0.550  
Calculated sin(theta\_max)/wavelength = 0.3688

**Author Response: Despite long exposure times there was no observable signal past approximately 1.5Ang resolution.**

PLAT023\_ALERT\_3\_A Resolution (too) Low [sin(theta)/Lambda < 0.6].. 34.66 Deg.

**Author Response: Despite long exposure times there was no observable signal past approximately 1.5Ang resolution.**



#### Alert level B

Crystal system given = cubic

PLAT049_ALERT_1_B	Calculated Density less than 1.0 gcm-3 .....	0.2662
PLAT241_ALERT_2_B	Check High Ueq as Compared to Neighbors for	01
PLAT241_ALERT_2_B	Check High Ueq as Compared to Neighbors for	02
PLAT241_ALERT_2_B	Check High Ueq as Compared to Neighbors for	02
PLAT341_ALERT_3_B	Low Bond Precision on C-C Bonds .....	0.0191 Ang
PLAT372_ALERT_2_B	Short C(sp)-C(sp) Bond C14 - C15 ...	1.03 Ang.



#### Alert level C

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections too Low ....	45 Perc.
PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full Low .....	0.970
PLAT241_ALERT_2_C	Check High Ueq as Compared to Neighbors for	03
PLAT242_ALERT_2_C	Check Low Ueq as Compared to Neighbors for	01
PLAT242_ALERT_2_C	Check Low Ueq as Compared to Neighbors for	08
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ....	3.4
PLAT334_ALERT_2_C	Small Average Benzene C-C Dist. C1 -C3	1.36 Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C1 - C8 ...	1.56 Ang.



#### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	19
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained Atom Sites ....	19
PLAT004_ALERT_5_G	Info: Polymeric Structure Found with Dimension .	1
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF ....	?
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large.	0.12
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C1 -C3	0.19 Ang.
PLAT371_ALERT_2_G	Long C(sp2)-C(sp1) Bond C15 - C16 ...	1.56 Ang.
PLAT603_ALERT_4_G	Unit Cell TOO large for VOID SEARCH in Structure	!
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	26
	O2 -CU2 -O2 -C8 1.40 0.90 20.666 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	52
	C9 -C10 -C14 -C15 -86.10 1.30 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	53
	C9 -C10 -C14 -C15 86.10 1.30 119.656 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	54
	C10 -C14 -C15 -C16 180.00 3.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	56
	C14 -C15 -C16 -C17 -89.40 1.60 1.555 1.555 1.555	90.556
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	57
	C14 -C15 -C16 -C17 89.40 1.60 1.555 1.555 1.555	1.555
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.15 Ratio
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints .....	163
PLAT950_ALERT_5_G	Reported and Calculated Hmax Values Differ by ..	20

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3 **ALERT level A** = Most likely a serious problem - resolve or explain  
 6 **ALERT level B** = A potentially serious problem, consider carefully  
 8 **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  
 15 **ALERT type 2** Indicator that the structure model may be wrong or deficient  
 6 **ALERT type 3** Indicator that the structure quality may be low  
 8 **ALERT type 4** Improvement, methodology, query or suggestion  
 4 **ALERT type 5** Informative message, check

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## checkCIF publication errors

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### **Alert level A**

PUBL004\_ALERT\_1\_A The contact author's name and address are missing,  
     \_publ\_contact\_author\_name and \_publ\_contact\_author\_address.  
 PUBL005\_ALERT\_1\_A \_publ\_contact\_author\_email, \_publ\_contact\_author\_fax and  
     \_publ\_contact\_author\_phone are all missing.  
     At least one of these should be present.  
 PUBL006\_ALERT\_1\_A \_publ\_requested\_journal is missing  
     e.g. 'Acta Crystallographica Section C'  
 PUBL008\_ALERT\_1\_A \_publ\_section\_title is missing. Title of paper.  
 PUBL009\_ALERT\_1\_A \_publ\_author\_name is missing. List of author(s) name(s).  
 PUBL010\_ALERT\_1\_A \_publ\_author\_address is missing. Author(s) address(es).  
 PUBL012\_ALERT\_1\_A \_publ\_section\_abstract is missing.  
     Abstract of paper in English.

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### **Alert level G**

PUBL013\_ALERT\_1\_G The \_publ\_section\_comment (discussion of study) is  
     missing. This is required for a full paper submission (but is  
     optional for an electronic paper).  
 PUBL017\_ALERT\_1\_G The \_publ\_section\_references section is missing or  
     empty.

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7 **ALERT level A** = Data missing that is essential or data in wrong format  
 2 **ALERT level G** = General alerts. Data that may be required is missing

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## Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.

If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
```

PROBLEM: \_publ\_section\_abstract is missing.  
RESPONSE: ...  
;  
# end Validation Reply Form

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

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## PLATON version of 18/07/2011; check.def file version of 04/07/2011

Datablock I - ellipsoid plot

