

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: CU

Bond precision:	C-C = 0.0093 A	Wavelength=0.71073	
Cell:	a=10.7226 (16)	b=9.6646 (15)	c=21.695 (3)
	alpha=90	beta=104.187 (2)	gamma=90
Temperature:	213 K		
	Calculated	Reported	
Volume	2179.7 (6)	2179.7 (6)	
Space group	P 21/n	P 21/n	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C38 H36 Cu2 N16 O6 S4	C38 H36 Cu2 N16 O6 S4	
Sum formula	C38 H36 Cu2 N16 O6 S4	C38 H36 Cu2 N16 O6 S4	
Mr	1068.17	1068.15	
Dx, g cm ⁻³	1.628	1.627	
Z	2	2	
Mu (mm ⁻¹)	1.235	1.235	
F000	1092.0	1092.0	
F000'	1094.57		
h, k, lmax	13, 12, 27	13, 12, 27	
Nref	4444	4404	
Tmin, Tmax	0.929, 0.940	0.929, 0.940	
Tmin'	0.539		

Correction method= # Reported T Limits: Tmin=0.929 Tmax=0.940
AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 26.368

R(reflections)= 0.0677 (3194)	wR2(reflections)=
S = 1.048	0.1573 (4404)
Npar= 298	

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.

Alert level B

PLAT213_ALERT_2_B Atom C7 has ADP max/min Ratio 4.1 prolat

Alert level C

PLAT213_ALERT_2_C Atom C5 has ADP max/min Ratio 3.2 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.4 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O3 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C5 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C6 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C7 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N3 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00931 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C4 - C5 . 1.40 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C6 - C7 . 1.39 Ang.
PLAT761_ALERT_1_C CIF Contains no X-H Bonds Please Check
PLAT762_ALERT_1_C CIF Contains no X-Y-H or H-Y-H Angles Please Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C38 H36 Cu2 N16 O6 S4

Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 18.48 Why ?
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) . 2.19 Info
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

- 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
5 **ALERT level G** = General information/check it is not something unexpected
- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
13 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
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
-

checkCIF publication errors

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.



Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.

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

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 a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# 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
```

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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 you wish to submit your CIF for publication in IUCrData 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.

