**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](http://journals.iucr.org/services/cif/checking/checkcifreport.html)

**Datablock: s155\_sq**

Bond precision: C-C = 0.0095 A Wavelength=0.71073

|  |  |  |  |
| --- | --- | --- | --- |
| Cell: | a=11.4654(5) | b=12.0318(5) | c=16.5011(6) |
|  | alpha=107.797(3) | beta=94.373(3) | gamma=96.281(3) |
| Temperature: | 293 K |  |  |

Moiety formula

Cu N4 O), 8(H2 O) [+

solvent]

O32, 2(C24 H18

Cu N4 O), 8(H2 O)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Calculated |  |  | Reported |
| Volume | 2139.86(16) |  |  | 2139.86(16) |
| Space group | P -1 |  |  | P -1 |
| Hall group | -P 1 |  |  | -P 1 |
|  | C20 H20 Ge4 | O32, | 2(C24 H | 18 C20 H20 Ge4 |

C68 H72 Cu2 Ge4 N8 O42 [+

Sum formula

solvent] C68 H72 Cu2 Ge4 N8 O42

Mr 2090.88 2090.77

Dx,g cm-3 1.622 1.622

Z 1 1

Mu (mm-1) 1.973 1.973

F000 1058.0 1058.0

F000’ 1059.78

h,k,lmax 14,15,21 14,15,21

Nref 9824 9808

Tmin,Tmax 0.403,0.553 0.377,1.000

Tmin’ 0.359

Correction method= # Reported T Limits: Tmin=0.377 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 27.499

R(reflections)= 0.0594( 6514) wR2(reflections)= 0.1343( 9808) S = 0.993 Npar= 568

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**

[PLAT417\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT417.html) Short Inter D-H..H-D H1 ..H20B . 2.05 Ang. x,y,z = 1\_555 Check

[PLAT417\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT417.html) Short Inter D-H..H-D H16A ..H21B . 1.80 Ang.

-x,-y,1-z = 2\_556 Check [PLAT420\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT420.html) D-H Without Acceptor O18 --H18A . Please Check [PLAT420\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT420.html) D-H Without Acceptor O20 --H20A . Please Check [PLAT990\_ALERT\_1\_B](http://journals.iucr.org/services/cif/checking/PLAT990.html) Deprecated .res/.hkl Input Style SQUEEZE Job ... ! Note

**Alert level C**

[PLAT193\_ALERT\_1\_C](http://journals.iucr.org/services/cif/checking/PLAT193.html) Cell and Diffraction Temperatures Differ by .... 1 Degree [PLAT230\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT230.html) Hirshfeld Test Diff for N4 --C34 . 6.9 s.u. [PLAT241\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT241.html) High ’MainMol’ Ueq as Compared to Neighbors of C34 Check [PLAT250\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT250.html) Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.6 Note [PLAT260\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT260.html) Large Average Ueq of Residue Including O20 0.112 Check [PLAT341\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT341.html) Low Bond Precision on C-C Bonds ............... 0.0095 Ang.

**Alert level G**

[PLAT005\_ALERT\_5\_G](http://journals.iucr.org/services/cif/checking/PLAT005.html) No Embedded Refinement Details Found in the CIF Please Do ! [PLAT007\_ALERT\_5\_G](http://journals.iucr.org/services/cif/checking/PLAT007.html) Number of Unrefined Donor-H Atoms .............. 14 Report [PLAT093\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT093.html) No s.u.’s on H-positions, Refinement Reported as mixed Check [PLAT154\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT154.html) The s.u.’s on the Cell Angles are Equal ..(Note) 0.003 Degree [PLAT200\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT200.html) Reported \_diffrn\_ambient\_temperature ..... (K) 293 Check [PLAT432\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT432.html) Short Inter X...Y Contact O2 ..C11 3.01 Ang.

1-x,1-y,1-z = 2\_666 Check [PLAT606\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT606.html) VERY LARGE Solvent Accessible VOID(S) in Structure ! Info [PLAT790\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT790.html) Centre of Gravity not Within Unit Cell: Resd. # 6 Note

H2 O

[PLAT793\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT793.html) Model has Chirality at C2 (Centro SPGR) R Verify [PLAT793\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT793.html) Model has Chirality at C3 (Centro SPGR) R Verify [PLAT793\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT793.html) Model has Chirality at C4 (Centro SPGR) S Verify [PLAT793\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT793.html) Model has Chirality at C7 (Centro SPGR) R Verify [PLAT793\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT793.html) Model has Chirality at C8 (Centro SPGR) R Verify [PLAT793\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT793.html) Model has Chirality at C9 (Centro SPGR) S Verify [PLAT794\_ALERT\_5\_G](http://journals.iucr.org/services/cif/checking/PLAT794.html) Tentative Bond Valency for Cu1 (II) . 2.29 Info [PLAT869\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT869.html) ALERTS Related to the Use of SQUEEZE Suppressed ! Info

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

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

6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

16 **ALERT level G** = General information/check it is not something unexpected

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

9 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

9 ALERT type 4 Improvement, methodology, query or suggestion

3 ALERT type 5 Informative message, check

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](http://journals.iucr.org/services/cif/checking/checkform.html) 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.

**PLATON version of 22/04/2020; check.def file version of 09/03/2020**

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**Datablock** s -

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