**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: seyf120**

Bond precision: C-C = 0.0195 A Wavelength=0.71073

|  |  |  |  |
| --- | --- | --- | --- |
| Cell: | a=14.5962(10) | b=14.6740(9) | c=15.3992(10) |
|  | alpha=73.821(6) | beta=76.019(6) | gamma=82.003(6) |
| Temperature: | 294 K |  |  |

Calculated Reported Volume 3064.7(4) 3064.7(4) Space group P -1 P -1

Hall group -P 1 -P 1

Moiety formula C20 H20 Ge4 O32, 4(C24 H16 C20 H20 Ge4 O32, 4(C24 H16

Cl Cu N4), 8(H2 O)

Sum formula C116 H100 Cl4 Cu4 Ge4 N16

O40

Cl Cu N4), 8(H2 O)

C116 H100 Cl4 Cu4 Ge4 N16

O40

Mr 3044.56 3044.43

Dx,g cm-3 1.650 1.650

Z 1 1

Mu (mm-1) 1.826 1.826

F000 1540.0 1540.0

F000’ 1543.10

h,k,lmax 17,18,18 17,18,18

Nref 12033 12002

|  |  |  |
| --- | --- | --- |
| Tmin,Tmax | 0.420,0.578 | 0.480,1.000 |
| Tmin’ | 0.331 |  |

Correction method= # Reported T Limits: Tmin=0.480 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 25.999

R(reflections)= 0.0986( 4973) wR2(reflections)= 0.2693( 12002) S = 0.986 Npar= 831

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**

[PLAT341\_ALERT\_3\_B](http://journals.iucr.org/services/cif/checking/PLAT341.html) Low Bond Precision on C-C Bonds ............... 0.0195 Ang. [PLAT417\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT417.html) Short Inter D-H..H-D H19A ..H20A . 1.85 Ang.

2-x,-y,2-z = 2\_757 Check [PLAT420\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT420.html) D-H Without Acceptor O1 --H1 . Please Check [PLAT420\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT420.html) D-H Without Acceptor O20 --H20A . Please Check [PLAT420\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT420.html) D-H Without Acceptor O20 --H20B . Please Check

**Alert level C**

[RINTA01\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/RINTA_01.html) The value of Rint is greater than 0.12

Rint given 0.126

[PLAT020\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT020.html) The Value of Rint is Greater Than 0.12 ......... 0.126 Report [PLAT026\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT026.html) Ratio Observed / Unique Reflections (too) Low .. 41% Check [PLAT084\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT084.html) High wR2 Value (i.e. > 0.25) ................... 0.27 Report [PLAT220\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT220.html) NonSolvent Resd 1 O Ueq(max) / Ueq(min) Range 3.7 Ratio [PLAT230\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT230.html) Hirshfeld Test Diff for Ge1 --O4 . 5.2 s.u. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference O2 --C1 . 0.17 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference O7 --C5 . 0.17 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference O10 --C6 . 0.18 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference O11 --C7 . 0.22 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference O12 --C8 . 0.18 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference C3 --C4 . 0.19 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference C9 --C10 . 0.19 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference N3 --C27 . 0.17 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference C0AA --C17 . 0.19 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference C18 --C20 . 0.19 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference C26 --C28 . 0.20 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference C28 --C29 . 0.25 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference C30 --C31 . 0.25 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference C30 --C32 . 0.24 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference N7 --C51 . 0.20 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference C50 --C52 . 0.17 Ang. [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) Large Hirshfeld Difference C53 --C54 . 0.19 Ang. [PLAT241\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT241.html) High ’MainMol’ Ueq as Compared to Neighbors of C21 Check [PLAT241\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT241.html) High ’MainMol’ Ueq as Compared to Neighbors of C53 Check [PLAT241\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT241.html) High ’MainMol’ Ueq as Compared to Neighbors of C56 Check [PLAT242\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of C1 Check [PLAT242\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of C9 Check [PLAT242\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of C50 Check [PLAT250\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT250.html) Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.2 Note [PLAT260\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT260.html) Large Average Ueq of Residue Including O18 0.104 Check [PLAT260\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT260.html) Large Average Ueq of Residue Including O19 0.256 Check [PLAT260\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT260.html) Large Average Ueq of Residue Including O20 0.192 Check [PLAT414\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT414.html) Short Intra D-H..H-X H5 ..H9 1.92 Ang.

x,y,z = 1\_555 Check

[PLAT417\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT417.html) Short Inter D-H..H-D H16 ..H17A . 2.14 Ang. x,y,z = 1\_555 Check

[PLAT601\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT601.html) Structure Contains Solvent Accessible VOIDS of . 74 Ang\*\*3

**Alert level G**

[PLAT002\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT002.html) Number of Distance or Angle Restraints on AtSite 10 Note [PLAT003\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT003.html) Number of Uiso or Uij Restrained non-H Atoms ... 7 Report [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 .............. 12 Report

[PLAT154\_ALERT\_1\_G](http://journals.iucr.org/services/cif/checking/PLAT154.html) The s.u.’s on the Cell Angles are Equal ..(Note) 0.006 Degree [PLAT335\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT335.html) Check Large C6 Ring C-C Range C26 -C28 0.17 Ang. [PLAT432\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT432.html) Short Inter X...Y Contact Cl2 ..C20 3.23 Ang.

x,1+y,-1+z = 1\_564 Check [PLAT720\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT720.html) Number of Unusual/Non-Standard Labels .......... 2 Note [PLAT790\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT790.html) Centre of Gravity not Within Unit Cell: Resd. # 2 Note

C24 H16 Cl Cu N4

[PLAT790\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT790.html) Centre of Gravity not Within Unit Cell: Resd. # 4 Note

H2 O

[PLAT790\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT790.html) Centre of Gravity not Within Unit Cell: Resd. # 5 Note

H2 O

[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) . 2.24 Info [PLAT794\_ALERT\_5\_G](http://journals.iucr.org/services/cif/checking/PLAT794.html) Tentative Bond Valency for Cu2 (II) . 2.23 Info [PLAT860\_ALERT\_3\_G](http://journals.iucr.org/services/cif/checking/PLAT860.html) Number of Least-Squares Restraints ............. 50 Note

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

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

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

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

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

23 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

28 ALERT type 4 Improvement, methodology, query or suggestion

4 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**

**Datablock seyfl20 - ellipsoid plot**

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z -143 se f120 p -1 R = 0. 10 RES=