**checkCIF/PLATON report**

Structure factors have been supplied for datablock(s) seyf63\_sq

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: seyf63\_sq**

Bond precision: C-C = 0.0248 A Wavelength=0.71073

|  |  |  |
| --- | --- | --- |
| Cell: | a=13.9136(12) | b=13.9818(13) c=15.1313(16) |
|  | alpha=113.398(10) | beta=106.248(8) gamma=94.594(7) |
| Temperature: | 294 K |  |

Calculated Reported Volume 2531.8(5) 2531.8(5) Space group P -1 P -1

Hall group -P 1 -P 1

C20 H20 Ge4 O32, 2(C36 H24 C20 H20 Ge4 O32, 2(C36 H24

Moiety formula

Cu N6), 8(H2 O) [+

solvent]

Cu N6), 8(H2 O)

C92 H84 Cu2 Ge4 N12 O40 [+

Sum formula

solvent] C92 H84 Cu2 Ge4 N12 O40

Mr 2415.25 2415.15

Dx,g cm-3 1.584 1.584

Z 1 1

Mu (mm-1) 1.680 1.680

F000 1226.0 1226.0

F000’ 1227.82

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

Nref 9971 9958

Tmin,Tmax 0.451,0.715 0.098,1.000

Tmin’ 0.361

Correction method= # Reported T Limits: Tmin=0.098 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.998

R(reflections)= 0.1081( 3217) wR2(reflections)= 0.2444( 9958) S = 0.951 Npar= 670

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**

[RINTA01\_ALERT\_3\_B](http://journals.iucr.org/services/cif/checking/RINTA_01.html) The value of Rint is greater than 0.18

Rint given 0.188

[PLAT020\_ALERT\_3\_B](http://journals.iucr.org/services/cif/checking/PLAT020.html) The Value of Rint is Greater Than 0.12 ......... 0.188 Report [PLAT026\_ALERT\_3\_B](http://journals.iucr.org/services/cif/checking/PLAT026.html) Ratio Observed / Unique Reflections (too) Low .. 32% Check [PLAT341\_ALERT\_3\_B](http://journals.iucr.org/services/cif/checking/PLAT341.html) Low Bond Precision on C-C Bonds ............... 0.02477 Ang. [PLAT417\_ALERT\_2\_B](http://journals.iucr.org/services/cif/checking/PLAT417.html) Short Inter D-H..H-D H16A ..H17B . 1.94 Ang.

1-x,-y,1-z = 2\_656 Check [PLAT910\_ALERT\_3\_B](http://journals.iucr.org/services/cif/checking/PLAT910.html) Missing # of FCF Reflection(s) Below Theta(Min). 13 Note [PLAT990\_ALERT\_1\_B](http://journals.iucr.org/services/cif/checking/PLAT990.html) Deprecated .res/.hkl Input Style SQUEEZE Job ... ! Note

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  **Alert level**[PLAT082\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT082.html) | **C**High R | 1 Value | .................................. | 0.11 | Report |
| [PLAT213\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT213.html) | Atom C | 6 | has ADP max/min Ratio ..... | 3.2 | prolat |
| [PLAT213\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT213.html) | Atom C | 7 | has ADP max/min Ratio ..... | 3.5 | prolat |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | O2 | --C1 | . | 0.20 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | O3 | --C1 | . | 0.19 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | O8 | --C5 | . | 0.18 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | O9 | --C6 | . | 0.21 | 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 | Cu1 | --N3 | . | 0.16 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | Cu1 | --N5 | . | 0.19 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | N1 | --C11 | . | 0.21 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | N2 | --C22 | . | 0.22 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | N3 | --C23 | . | 0.19 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | C14 | --C16 | . | 0.25 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | C16 | --C17 | . | 0.23 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | C18 | --C19 | . | 0.17 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | C18 | --C20 | . | 0.21 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | C20 | --C21 | . | 0.21 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | C21 | --C22 | . | 0.21 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | C29 | --C30 | . | 0.23 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | C30 | --C31 | . | 0.23 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | C38 | --C39 | . | 0.19 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | C42 | --C43 | . | 0.22 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | C42 | --C44 | . | 0.22 | Ang. |
| [PLAT234\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT234.html) | Large | Hirshfeld | Difference | C44 | --C45 | . | 0.24 | Ang. |

[PLAT241\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT241.html) High ’MainMol’ Ueq as Compared to Neighbors of C17 Check

[PLAT242\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT242.html) Low ’MainMol’ Ueq as Compared to Neighbors of C6 Check [PLAT260\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT260.html) Large Average Ueq of Residue Including O17 0.115 Check [PLAT260\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT260.html) Large Average Ueq of Residue Including O18 0.109 Check [PLAT260\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT260.html) Large Average Ueq of Residue Including O19 0.123 Check [PLAT260\_ALERT\_2\_C](http://journals.iucr.org/services/cif/checking/PLAT260.html) Large Average Ueq of Residue Including O20 0.106 Check [PLAT790\_ALERT\_4\_C](http://journals.iucr.org/services/cif/checking/PLAT790.html) Centre of Gravity not Within Unit Cell: Resd. # 1 Note

C20 H20 Ge4 O32

[PLAT906\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT906.html) Large K Value in the Analysis of Variance ...... 51.845 Check [PLAT906\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT906.html) Large K Value in the Analysis of Variance ...... 3.848 Check [PLAT906\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT906.html) Large K Value in the Analysis of Variance ...... 11.245 Check [PLAT906\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT906.html) Large K Value in the Analysis of Variance ...... 2.797 Check [PLAT906\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT906.html) Large K Value in the Analysis of Variance ...... 5.678 Check [PLAT906\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT906.html) Large K Value in the Analysis of Variance ...... 2.058 Check [PLAT906\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT906.html) Large K Value in the Analysis of Variance ...... 3.359 Check [PLAT906\_ALERT\_3\_C](http://journals.iucr.org/services/cif/checking/PLAT906.html) Large K Value in the Analysis of Variance ...... 2.195 Check

**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 .............. 12 Report [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. # 2 Note

C36 H24 Cu N6

[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) S Verify [PLAT793\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT793.html) Model has Chirality at C3 (Centro SPGR) S Verify [PLAT793\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT793.html) Model has Chirality at C4 (Centro SPGR) R 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 (I) . 1.18 Info [PLAT869\_ALERT\_4\_G](http://journals.iucr.org/services/cif/checking/PLAT869.html) ALERTS Related to the Use of SQUEEZE Suppressed ! Info [PLAT913\_ALERT\_3\_G](http://journals.iucr.org/services/cif/checking/PLAT913.html) Missing # of Very Strong Reflections in FCF .... 1 Note [PLAT961\_ALERT\_5\_G](http://journals.iucr.org/services/cif/checking/PLAT961.html) Dataset Contains no Negative Intensities ....... Please Check [PLAT978\_ALERT\_2\_G](http://journals.iucr.org/services/cif/checking/PLAT978.html) Number C-C Bonds with Positive Residual Density. 0 Info

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

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

40 **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

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

11 ALERT type 2 Indicator that the structure model may be wrong or deficient

14 ALERT type 3 Indicator that the structure quality may be low

34 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 sey -

- - - - NOMO

**f63 sq - ellipsoid plot**

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se f63\_s

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R = 0. 11 RES=