

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 5, 6, 7

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: 5

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Bond precision:	C-C = 0.0042 Å	Wavelength=0.71073	
Cell:	a=10.3934(6)	b=15.3160(9)	c=18.0563(11)
	alpha=90	beta=90	gamma=90
Temperature:	193 K		
	Calculated	Reported	
Volume	2874.3(3)	2874.3(3)	
Space group	P 21 21 21	P 21 21 21	
Hall group	P 2ac 2ab	P 2ac 2ab	
Moiety formula	C27 H33 Cl2 Ge N2 O P S	?	
Sum formula	C27 H33 Cl2 Ge N2 O P S	C27 H33 Cl2 Ge N2 O P S	
Mr	608.09	608.07	
Dx,g cm-3	1.405	1.405	
Z	4	4	
Mu (mm-1)	1.403	1.403	
F000	1256.0	1256.0	
F000'	1258.97		
h,k,lmax	13,20,24	13,20,24	
Nref	7158[ 4001]	7146	
Tmin,Tmax	0.721,0.799	0.616,0.746	
Tmin'	0.519		

Correction method= # Reported T Limits: Tmin=0.616 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 1.79/1.00      Theta(max)= 28.319

R(reflections)= 0.0291( 6501)      wR2(reflections)= 0.0561( 7146)

S = 1.070      Npar= 320

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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.



### Alert level C

PLAT910\_ALERT\_3\_C Missing # of FCF Reflection(s) Below Theta(Min).

8 Note



### Alert level G

PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary .

Please Do !

PLAT913\_ALERT\_3\_G Missing # of Very Strong Reflections in FCF ....

1 Note

PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density.

7 Info

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 0 **ALERT level B** = A potentially serious problem, consider carefully  
 1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 3 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 1 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 2 ALERT type 3 Indicator that the structure quality may be low  
 0 ALERT type 4 Improvement, methodology, query or suggestion  
 0 ALERT type 5 Informative message, check
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## Datablock: 6

Bond precision: C-C = 0.0033 A

Wavelength=0.71073

Cell: a=11.2219(5) b=18.1701(7) c=15.7026(6)

alpha=90

beta=93.4488(15)

gamma=90

Temperature: 193 K

	Calculated	Reported
Volume	3196.0(2)	3196.0(2)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C27 H33 Cl4 Ge2 N2 O P S	?
Sum formula	C27 H33 Cl4 Ge2 N2 O P S	C27 H33 Cl4 Ge2 N2 O P S
Mr	751.60	751.56
Dx,g cm-3	1.562	1.562
Z	4	4
Mu (mm-1)	2.355	2.355
F000	1520.0	1520.0
F000'	1524.76	
h,k,lmax	16,25,22	16,25,22
Nref	9811	9769
Tmin,Tmax	0.574,0.754	0.651,0.746
Tmin'	0.405	

Correction method= # Reported T Limits: Tmin=0.651 Tmax=0.746

AbsCorr = MULTI-SCAN

Data completeness= 0.996

Theta(max)= 30.561

R(reflections)= 0.0306( 7740)

wR2(reflections)= 0.0741( 9769)

S = 1.029

Npar= 347

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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.



#### Alert level B

PLAT230\_ALERT\_2\_B Hirshfeld Test Diff for Ge1 --Ge2 . 14.1 s.u.  
PLAT910\_ALERT\_3\_B Missing # of FCF Reflection(s) Below Theta(Min). 11 Note



#### Alert level C

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.6 Ratio



#### Alert level G

PLAT432\_ALERT\_2\_G Short Inter X...Y Contact O1 ..C24 2.96 Ang.  
1-x,1-y,1-z = 3\_666 Check  
PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 31 Note  
PLAT913\_ALERT\_3\_G Missing # of Very Strong Reflections in FCF .... 2 Note  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 10 Info

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1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
4 ALERT type 2 Indicator that the structure model may be wrong or deficient  
2 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
0 ALERT type 5 Informative message, check

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## Datablock: 7

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Bond precision: C-C = 0.0055 A

Wavelength=0.71073

Cell: a=9.0496(12) b=14.5792(16) c=22.036(3)

alpha=90 beta=90.653(4) gamma=90

Temperature: 193 K

	Calculated	Reported
Volume	2907.2(6)	2907.2(6)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C27 H33 Cl2 Ge N2 O P S	?
Sum formula	C27 H33 Cl2 Ge N2 O P S	C27 H33 Cl2 Ge N2 O P S
Mr	608.09	608.07
Dx,g cm-3	1.389	1.389
Z	4	4
Mu (mm-1)	1.387	1.387
F000	1256.0	1256.0
F000'	1258.97	
h,k,lmax	11,18,27	11,18,27
Nref	5938	5915
Tmin,Tmax	0.905,0.973	0.672,0.719
Tmin'	0.870	

Correction method= # Reported T Limits: Tmin=0.672 Tmax=0.719  
AbsCorr = MULTI-SCAN

Data completeness= 0.996                      Theta(max)= 26.371

R(reflections)= 0.0456( 3770)              wR2(reflections)= 0.0916( 5915)

S = 1.030                                      Npar= 320

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

PLAT910\_ALERT\_3\_B Missing # of FCF Reflection(s) Below Theta(Min). 11 Note



#### Alert level C

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12

Rint given 0.149

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 13 Report



#### Alert level G

PLAT020\_ALERT\_3\_G The Value of Rint is Greater Than 0.12 ..... 0.149 Report

PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !

PLAT913\_ALERT\_3\_G Missing # of Very Strong Reflections in FCF .... 2 Note

PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 16 Note

PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 3 Info

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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 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.

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**PLATON version of 05/12/2020; check.def file version of 05/12/2020**





