

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

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Bond precision:    C-C = 0.0065 Å                      Wavelength=0.71073

Cell:                      a=8.5100 (17)              b=11.680 (2)              c=21.020 (4)  
                            alpha=84.47 (3)              beta=85.62 (3)              gamma=83.13 (3)

Temperature:            100 K

	Calculated	Reported
Volume	2060.2 (7)	2060.2 (7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C48 H28 F10 Hg O3 P2	C48 H28 F10 Hg O3 P2
Sum formula	C48 H28 F10 Hg O3 P2	C48 H28 F10 Hg O3 P2
Mr	1105.24	1105.23
Dx, g cm <sup>-3</sup>	1.782	1.782
Z	2	2
Mu (mm <sup>-1</sup> )	3.903	3.903
F000	1080.0	1080.0
F000'	1076.34	
h, k, lmax	11, 15, 28	11, 15, 28
Nref	11053	8939
Tmin, Tmax	0.684, 0.732	
Tmin'	0.670	

Correction method= Not given

Data completeness= 0.809                      Theta(max)= 29.094

R(reflections)= 0.0376 ( 7792)

wR2(reflections)=  
0.1078 ( 8939)

S = 1.060

Npar= 577

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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.

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### Alert level C

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 100 Report

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### Alert level G

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
not performed for this radiation type.

PLAT154\_ALERT\_1\_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.03 Degree

PLAT180\_ALERT\_4\_G Check Cell Rounding: # of Values Ending with 0 = 3 Note

PLAT434\_ALERT\_2\_G Short Inter HL..HL Contact F5 ..F5 . 2.80 Ang.

1-x,1-y,2-z = 2\_667 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 2014 Note

PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 3 Note

PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 4.6 Low

PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 0 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

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

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

3 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

2 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

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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.

