

# 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

## Datablock: I

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Bond precision:	N- C = 0.0148 A	Wavelength=0.71073
Cell:	a=3.7089(5)	b=6.4098(6)      c=8.150(6)
	alpha=81.575(6)	beta=80.379(7)      gamma=80.195(7)
Temperature:	100 K	
	Calculated	Reported
Volume	186.84(14)	186.84(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C2 Hg N3	2(C2 N3), 2(Hg)
Sum formula	C2 Hg N3	C4 Hg2 N6
Mr	266.64	533.30
Dx,g cm-3	4.740	4.739
Z	2	1
Mu (mm-1)	40.978	41.090
F000	226.0	226.0
F000'	221.92	
h,k,lmax	5,10,12	5,9,12
Nref	1519	1263
Tmin,Tmax	0.027,0.440	0.067,0.673
Tmin'	0.001	

Correction method= # Reported T Limits: Tmin=0.067 Tmax=0.673  
AbsCorr = GAUSSIAN

Data completeness= 0.831      Theta(max)= 33.970

R(reflections)= 0.0468( 1154)      wR2(reflections)= 0.1091( 1263)

S = 3.600      Npar= 55

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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

GOODF01\_ALERT\_2\_C The least squares goodness of fit parameter lies  
outside the range 0.80 <> 2.00  
Goodness of fit given = 3.600

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### Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..		Please Check
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	2.00	Check
PLAT982_ALERT_1_G	The Hg-f' = -2.444 Deviates from IT-value =	-2.389	Check
PLAT983_ALERT_1_G	The Hg-f" = 9.373 Deviates from IT-Value =	9.227	Check

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

5 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  
0 ALERT type 3 Indicator that the structure quality may be low  
0 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

Datablock I - ellipsoid plot

