

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2

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: 2

Bond precision:	C-C = 0.0094 Å	Wavelength=0.71073
Cell:	a=9.1384(5)	b=11.7625(8) c=12.7526(7)
	alpha=90	beta=92.798(5) gamma=90
Temperature:	170 K	
	Calculated	Reported
Volume	1369.15(14)	1369.15(14)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C12 H9 Cl Hg N2 O4	?
Sum formula	C12 H9 Cl Hg N2 O4	C12 H9 Cl Hg N2 O4
Mr	481.25	481.25
Dx,g cm-3	2.335	2.335
Z	4	4
Mu (mm-1)	11.450	11.450
F000	896.0	896.0
F000'	887.95	
h,k,lmax	10,13,15	10,13,15
Nref	2402	2401
Tmin,Tmax		0.359,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.359 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 24.997

R(reflections)= 0.0325(2070) wR2(reflections)= 0.0804(2401)

S = 1.117 Npar= 184

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

PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...	Please Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0094 Ang.
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.07A From Hg1	1.75 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.15A From Hg1	1.72 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.96A From O3	1.07 eA-3

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2 Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1 Report
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	1 Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	73% Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.9 Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
7 **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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 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

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT053_2
;
PROBLEM: Minimum Crystal Dimension Missing (or Error) ...      Please Check
RESPONSE: ...
;
_vrf_PLAT054_2
;
PROBLEM: Medium Crystal Dimension Missing (or Error) ...      Please Check
RESPONSE: ...
;
_vrf_PLAT055_2
;
PROBLEM: Maximum Crystal Dimension Missing (or Error) ...      Please Check
RESPONSE: ...
;
_vrf_PLAT342_2
;
PROBLEM: Low Bond Precision on C-C Bonds .....                0.0094 Ang.
RESPONSE: ...
;
_vrf_PLAT971_2
;
```

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PROBLEM: Check Calcd Resid. Dens.  1.07A   From Hg1          1.75 eA-3
RESPONSE: ...
;
_vrf_PLAT975_2
;
PROBLEM: Check Calcd Resid. Dens.  0.96A   From O3          1.07 eA-3
RESPONSE: ...
;
# end Validation Reply Form
```

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.

PLATON version of 03/06/2021; check.def file version of 02/06/2021

