

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: hadi1001_0m

Bond precision: C-C = 0.0077 A Wavelength=0.71073

Cell: a=8.1781(4) b=15.7816(8) c=13.7018(7)
 alpha=90 beta=97.020(2) gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	1755.15(15)	1755.15(15)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	?
Moiety formula	C19 H14 N2 O6	?
Sum formula	C19 H14 N2 O6	C19 H14 N2 O6
Mr	366.32	366.32
Dx,g cm-3	1.386	1.386
Z	4	4
Mu (mm-1)	0.105	0.105
F000	760.0	760.0
F000'	760.43	
h,k,lmax	9,18,16	9,18,16
Nref	3084	3082
Tmin,Tmax	0.973,0.982	0.918,1.000
Tmin'	0.973	

Correction method= MULTI-SCAN

Data completeness= 0.999 Theta(max)= 24.990

R(reflections)= 0.0900(1994) wR2(reflections)= 0.2428(3082)

S = 1.056 Npar= 245

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

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for      O4      -- N1      ..      5.2 su
PLAT234_ALERT_4_C Large Hirshfeld Difference C10      -- C19      ..      0.20 Ang.
PLAT242_ALERT_2_C Check Low          Ueq as Compared to Neighbors for      N1
PLAT242_ALERT_2_C Check Low          Ueq as Compared to Neighbors for      N2
PLAT242_ALERT_2_C Check Low          Ueq as Compared to Neighbors for      C10
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds .....      0.0077 Ang.
```

● Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF      ? Do !
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large.      0.13
PLAT128_ALERT_4_G Note: Alternate Setting of Space-group P21/c      .      P21/n
```

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 - 0 **ALERT level B** = A potentially serious problem, consider carefully
 - 6 **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
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- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 5 ALERT type 2 Indicator that the structure model may be wrong or deficient
 - 1 ALERT type 3 Indicator that the structure quality may be low
 - 2 ALERT type 4 Improvement, methodology, query or suggestion
 - 1 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*, 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 01/06/2013; check.def file version of 24/05/2013

Datablock hadi1001_0m - ellipsoid plot

