

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: p14

Bond precision: C-C = 0.0015 Å Wavelength=1.54184

Cell: a=8.89574(10) b=9.41743(14) c=13.3599(2)
 alpha=75.4592(13) beta=77.5237(11) gamma=87.4987(11)
Temperature: 120 K

	Calculated	Reported
Volume	1057.73(3)	1057.73(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C29 H26 N2 O	C29 H26 N2 O
Sum formula	C29 H26 N2 O	C29 H26 N2 O
Mr	418.52	418.52
Dx, g cm ⁻³	1.314	1.314
Z	2	2
Mu (mm ⁻¹)	0.619	0.619
F000	444.0	444.0
F000'	445.20	
h, k, lmax	11, 12, 17	11, 12, 17
Nref	4612	4554
Tmin, Tmax	0.881, 0.952	
Tmin'	0.878	

Correction method= Not given

Data completeness= 0.987 Theta(max)= 79.873

R(reflections)= 0.0396(4251)	wR2(reflections)=
S = 1.073	0.1135(4554)
Npar= 290	

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

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 3.77 Report

PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 0.62 eA-3



Alert level G

PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF Please Check

PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum Found in CIF Please Check

PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C7 -C14 . 1.45 Ang.

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.9 Low

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **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
1 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
-

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_DIFMX02_p14
;
PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_PLAT094_p14
;
PROBLEM: Ratio of Maximum / Minimum Residual Density .... 3.77 Report
RESPONSE: ...
;
_vrf_PLAT097_p14
;
PROBLEM: Large Reported Max. (Positive) Residual Density 0.62 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.

