

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: dpa2_auto

Bond precision: C-C = 0.0050 Å Wavelength=0.71073

Cell: a=9.8515 (8) b=12.0994 (10) c=13.5043 (10)
 alpha=70.355 (7) beta=81.809 (7) gamma=66.735 (8)
Temperature: 293 K

	Calculated	Reported
Volume	1392.6 (2)	1392.6 (2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C37 H26 N4	C37 H26 N4
Sum formula	C37 H26 N4	C37 H26 N4
Mr	526.62	526.62
Dx, g cm ⁻³	1.256	1.256
Z	2	2
Mu (mm ⁻¹)	0.075	0.075
F000	552.0	552.0
F000'	552.19	
h, k, lmax	11, 14, 16	11, 14, 16
Nref	4922	4885
Tmin, Tmax		0.336, 1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.336 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.992 Theta(max)= 25.027

R(reflections)= 0.0760 (2747)	wR2(reflections)=
S = 1.080	0.2335 (4885)
Npar= 370	

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
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.22 Report
PLAT230_ALERT_2_C	Hirshfeld Test Diff for N002 --C005 .	6.0 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for N004 --C00J .	6.0 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C00E --C00H .	7.0 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C00K --C015 .	5.7 s.u.
PLAT331_ALERT_2_C	Small Aver Phenyl C-C Dist C00C --C00V .	1.37 Ang.
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.005 Ang.



Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	4 Report
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.12 Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	67 Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	2 Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
10 **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
8 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
1 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

