

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

Bond precision: C-C = 0.0047 Å Wavelength=0.71073

Cell: a=10.4403(13) b=21.619(3) c=25.312(3)
 alpha=90 beta=100.287(3) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	5621.3(12)	5621.2(12)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C36 H20 N4	C36 H20 N4
Sum formula	C36 H20 N4	C36 H20 N4
Mr	508.56	508.56
Dx,g cm-3	1.202	1.202
Z	8	8
Mu (mm-1)	0.072	0.072
F000	2112.0	2112.0
F000'	2112.73	
h,k,lmax	12,25,30	12,25,30
Nref	10022	10008
Tmin,Tmax	0.975,0.980	0.898,0.908
Tmin'	0.975	

Correction method= # Reported T Limits: Tmin=0.898 Tmax=0.908
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.099

R(reflections)= 0.0593(5296) wR2(reflections)= 0.1756(10008)

S = 1.004 Npar= 709

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 B

PLAT220_ALERT_2_B Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range 8.7 Ratio

Alert level C

PLAT018_ALERT_1_C _diffn_measured_fraction_theta_max .NE. *_full ! Check
PLAT213_ALERT_2_C Atom C70 has ADP max/min Ratio 3.1 prolat
PLAT213_ALERT_2_C Atom C71 has ADP max/min Ratio 3.1 prolat
PLAT213_ALERT_2_C Atom C72 has ADP max/min Ratio 3.1 prolat
PLAT222_ALERT_3_C Non-Solv. Resd 2 H Uiso(max)/Uiso(min) Range 8.7 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C67 --C68 . 5.9 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C68 --C69 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C69 --C70 . 0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C70 --C71 . 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C71 --C72 . 0.21 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C62 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C70 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C71 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C72 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C67 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.0047 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -2.949 Report
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 8 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.597 6 Report

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for C2 --C3 . 6.5 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for C64 --C65 . 7.0 s.u.
PLAT343_ALERT_2_G Unusual sp3 Angle Range in Main Residue for C4 Check
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C10 - C11 . 1.43 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C12 - C13 . 1.44 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C28 - C29 . 1.44 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C30 - C31 . 1.43 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C46 - C47 . 1.43 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C48 - C49 . 1.44 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C64 - C65 . 1.42 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C66 - C67 . 1.46 Ang.
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 !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 6 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
19 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
17 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
24 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
0 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* 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.

