

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SY_250K_0m

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: SY_250K_0m

Bond precision: C-C = 0.0034 Å Wavelength=1.54178

Cell: $a=9.4456(2)$ $b=18.6220(5)$ $c=9.8660(3)$
 $\alpha=90$ $\beta=94.2185(17)$ $\gamma=90$
Temperature: 250 K

	Calculated	Reported
Volume	1730.69(8)	1730.69(8)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C40 H48 N2 O2	?
Sum formula	C40 H48 N2 O2	C40 H48 N2 O2
Mr	588.80	588.80
Dx, g cm ⁻³	1.130	1.130
Z	2	2
Mu (mm ⁻¹)	0.529	0.529
F000	636.0	636.0
F000'	637.68	
h,k,lmax	11,22,11	11,22,11
Nref	3062	3048
Tmin,Tmax	0.938,0.948	
Tmin'	0.900	

Correction method= Not given

Data completeness= 0.995 Theta(max)= 66.572

R(reflections) = 0.0621(2103) wR2(reflections) = 0.1884(3048)

S = 1.098 Npar= 199

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

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT242_ALERT_2_C	Low MainMol Ueq as Compared to Neighbors of		C13 Check
PLAT242_ALERT_2_C	Low MainMol Ueq as Compared to Neighbors of		C17 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		3.391 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595	14 Report

🟢 Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	22	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	17	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	281	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	46%	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	1	Check

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
- 0 **ALERT level B** = A potentially serious problem, consider carefully
- 5 **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

- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
- 4 ALERT type 2 Indicator that the structure model may be wrong or deficient
- 4 ALERT type 3 Indicator that the structure quality may be low
- 3 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* 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 22/12/2019; check.def file version of 13/12/2019

Datablock SY_250K_0m - ellipsoid plot

