

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 = 0.0032 Å	Wavelength=0.71073	
Cell:	a=17.274(2)	b=17.574(2)	c=17.610(2)
	alpha=90	beta=119.159(2)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	4668.4(9)	4668.7(10)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C29 H25 N O2	?	
Sum formula	C29 H25 N O2	C58 H50 N2 O4	
Mr	419.50	839.00	
Dx, g cm ⁻³	1.194	1.194	
Z	8	4	
Mu (mm ⁻¹)	0.074	0.074	
F000	1776.0	1776.0	
F000'	1776.74		
h,k,lmax	20,20,20	20,20,20	
Nref	8216	8195	
Tmin,Tmax	0.981,0.982		
Tmin'	0.981		

Correction method= Not given

Data completeness= 0.997 Theta(max)= 25.000

R(reflections)= 0.0476(4844) wR2(reflections)= 0.1258(8195)

S = 0.811 Npar= 581

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

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	5.431	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	10	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.595	12	Report

● Alert level G

PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	2.00	Check
PLAT371_ALERT_2_G	Long C(sp2)-C(sp1) Bond C6 - C7 .	1.44	Ang.
PLAT371_ALERT_2_G	Long C(sp2)-C(sp1) Bond C8 - C9 .	1.44	Ang.
PLAT371_ALERT_2_G	Long C(sp2)-C(sp1) Bond C35 - C36 .	1.44	Ang.
PLAT371_ALERT_2_G	Long C(sp2)-C(sp1) Bond C37 - C38 .	1.43	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	1	Note
PLAT793_ALERT_4_G	Model has Chirality at C15 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C16 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	Model has Chirality at C17 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	Model has Chirality at C18 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	Model has Chirality at C44 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	Model has Chirality at C45 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C46 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C47 (Centro SPGR)	S	Verify
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 ...	12	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.8	Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities	Please	Check
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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- 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
20 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
9 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.

