

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: ic21784

Bond precision:	C-C = 0.0022 A		Wavelength=1.54178
Cell:	a=16.4711(10)	b=9.1373(6)	c=25.0870(15)
	alpha=90	beta=106.575(3)	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	3618.7(4)	3618.7(4)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C50 H42 O	?
Sum formula	C50 H42 O	C50 H42 O
Mr	658.84	658.83
Dx, g cm ⁻³	1.209	1.209
Z	4	4
Mu (mm ⁻¹)	0.534	0.534
F000	1400.0	1400.0
F000'	1403.65	
h, k, lmax	20, 11, 31	20, 11, 31
Nref	7794	7628
Tmin, Tmax	0.950, 0.989	0.812, 1.000
Tmin'	0.830	

Correction method= # Reported T Limits: Tmin=0.812 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.979 Theta (max)= 78.600

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R(reflections)= 0.0487( 6196)      wR2(reflections)=
S = 1.051                        0.1365( 7628)
Npar= 465
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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

PLAT411_ALERT_2_C Short Inter H...H Contact H9 ..H9 . 2.04 Ang.
1-x,2-y,1-z = 3_676 Check



Alert level G

PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O1 . 108.3 Degree
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check

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

- 1 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
0 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

