

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dm_skp_3_219_autored

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: dm_skp_3_219_autored

Bond precision:	C-C = 0.0025 A	Wavelength=0.71073
Cell:	a=4.9733(2)	b=15.3701(6) c=19.3784(9)
	alpha=90	beta=92.471(4) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	1479.91(11)	1479.91(11)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C18 H14 N2 O3	0.67(C18 H14 N2 O3)
Sum formula	C18 H14 N2 O3	C12 H9.33 N1.33 O2
Mr	306.31	204.21
Dx, g cm ⁻³	1.375	1.375
Z	4	6
Mu (mm ⁻¹)	0.095	0.095
F000	640.0	640.0
F000'	640.30	
h, k, lmax	7, 24, 30	7, 23, 30
Nref	5957	5498
Tmin, Tmax	0.993, 0.995	0.720, 1.000
Tmin'	0.989	

Correction method= # Reported T Limits: Tmin=0.720 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.923 Theta(max)= 33.802

R(reflections)= 0.0756(2689)	wR2(reflections)=
S = 1.034	0.1836(5498)
Npar= 209	

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

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.134

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.134 Report

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 49% Check

PLAT430_ALERT_2_C Short Inter D...A Contact 0002 ..0002 . 2.86 Ang.

2-x,-y,1-z = 3_756 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 32.090 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.061 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 6.711 Check



Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the

_chemical_formula_sum and _chemical_formula_moiety. This is usually due to the moiety formula being in the wrong format.

Atom count from _chemical_formula_sum: C12 H9.33 N1.33 O2

Atom count from _chemical_formula_moiety:C12.06 H9.38 N1.34 O2.01

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1 Report

PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ Please Check

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.6667 Check

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 37 Note

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 456 Note

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 9 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

7 **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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

2 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

2 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.

