

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision: C-C = 0.0027 Å Wavelength=1.54178

Cell: a=6.2275 (4) b=8.3963 (5) c=24.9490 (14)
 alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	1304.53 (14)	1304.53 (14)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C5 H8 N2 O3	C5 H8 N2 O3
Sum formula	C5 H8 N2 O3	C5 H8 N2 O3
Mr	144.13	144.13
Dx, g cm ⁻³	1.468	1.468
Z	8	8
Mu (mm ⁻¹)	1.050	1.050
F000	608.0	608.0
F000'	610.27	
h, k, lmax	7, 9, 29	7, 9, 28
Nref	2154 [1287]	2073
Tmin, Tmax	0.893, 0.919	0.810, 0.920
Tmin'	0.730	

Correction method= # Reported T Limits: Tmin=0.810 Tmax=0.920
AbsCorr = MULTI-SCAN

Data completeness= 1.61/0.96 Theta(max)= 63.730

R(reflections)= 0.0244 (2055)

wR2(reflections)=
0.0658 (2073)

S = 1.087

Npar= 185

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**

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5816
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) 6.92 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.582 6 Report
6 0 0, 7 2 0, 7 0 6, 7 1 6, 7 0 7, 0 2 28,

● **Alert level G**

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 4 Report
H1 H2A H4 H4D
PLAT480_ALERT_4_G Long H...A H-Bond Reported H7 ..05 . 2.61 Ang.
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 98% Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.23 Note
Predicted wR2: Based on SigI**2 2.04 or SHELX Weight 6.34
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

- 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
- 6 **ALERT level G** = General information/check it is not something unexpected

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 1 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
 - 1 ALERT type 4 Improvement, methodology, query or suggestion
 - 2 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.

Datablock I - ellipsoid plot

