

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: fa448

Bond precision: C-C = 0.0018 A

Wavelength=0.71073

Cell: a=5.2518(2) b=9.7329(5) c=10.3619(5)
 alpha=86.394(2) beta=79.737(2) gamma=79.631(2)
Temperature: 200 K

	Calculated	Reported
Volume	512.41(4)	512.41(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C9 H12 N2 O4	?
Sum formula	C9 H12 N2 O4	C9 H12 N2 O4
Mr	212.21	212.21
Dx,g cm-3	1.375	1.375
Z	2	2
Mu (mm-1)	0.109	0.109
F000	224.0	224.0
F000'	224.13	
h,k,lmax	7,12,13	6,12,13
Nref	2543	2530
Tmin,Tmax	0.974,0.995	
Tmin'	0.969	

Correction method= Not given

Data completeness= 0.995

Theta(max)= 28.320

R(reflections)= 0.0374(1997)

wR2(reflections)= 0.1050(2530)

S = 1.052

Npar= 137

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 A

EXPT005_ALERT_1_A _exptl_crystal_description is missing

Crystal habit description.

The following tests will not be performed.

CRYSR_01

DIFF003_ALERT_1_A _diffrn_measurement_device_type is missing

Diffractometer make and type. Replaces _diffrn_measurement_type.

PLAT015_ALERT_5_A No _shelx_hkl_file record in SHELXL20xy CIF Please Do !

PLAT183_ALERT_1_A Missing _cell_measurement_reflns_used value Please Do !

PLAT184_ALERT_1_A Missing _cell_measurement_theta_min value Please Do !

PLAT185_ALERT_1_A Missing _cell_measurement_theta_max value Please Do !

Alert level C

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree

PLAT432_ALERT_2_G Short Inter X...Y Contact O4 .. C2 .. 3.01 Ang.

PLAT432_ALERT_2_G Short Inter X...Y Contact C2 .. C5 .. 3.18 Ang.

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- 6 **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

- 7 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
0 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
3 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.

