

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) oh32r

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: oh32r

Bond precision:	C-C = 0.0030 A	Wavelength=0.71073
Cell:	a=7.9187(5) b=21.2234(13) c=5.0207(3)	
	alpha=90 beta=105.7360(19) gamma=90	
Temperature:	100 K	
	Calculated	Reported
Volume	812.16(9)	812.16(9)
Space group	P 21/c	?
Hall group	-P 2ybc	?
Moiety formula	C5 H6 N4 O3, 2(H2 O)	?
Sum formula	C5 H10 N4 O5	C10 H20 N8 O10
Mr	206.17	412.34
Dx,g cm-3	1.686	1.686
Z	4	2
Mu (mm-1)	0.150	0.150
F000	432.0	432.0
F000'	432.26	
h,k,lmax	9,25,5	9,25,5
Nref	1424	1422
Tmin,Tmax	0.991,0.997	0.929,0.997
Tmin'	0.928	

Correction method= # Reported T Limits: Tmin=0.929 Tmax=0.997
AbsCorr = ?

Data completeness= 0.999 Theta(max)= 25.020

R(reflections)= 0.0423(1039) wR2(reflections)= 0.0995(1422)

S = 1.020 Npar= 145

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

SYMM001_ALERT_1_A _symmetry_cell_setting is missing
The cell setting should be one of the following
* triclinic
* monoclinic
* orthorhombic
* tetragonal
* rhombohedral
* trigonal
* hexagonal
* cubic
The following tests will not be performed.
SYMMS_01, SYMMS_02
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.
PLAT122_ALERT_1_A No _symmetry_space_group_name_H-M Given 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

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.125
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT088_ALERT_3_C Poor Data / Parameter Ratio 9.81 Note
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 3.110 Check

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 3 Report
PLAT020_ALERT_3_G The value of Rint is greater than 0.12 0.125 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 2.00 Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT104_ALERT_1_G The Reported Crystal System is Inconsistent with P21/c Check
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) Still 61 %
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min) 2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density 2 Note

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- 7 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected
- 11 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
6 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.

