

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cxy3231_0m

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: cxy3231_0m

Bond precision:	C-C = 0.0051 A	Wavelength=1.54178	
Cell:	a=14.2104(3)	b=14.2104(3)	c=5.6788(2)
	alpha=90	beta=90	gamma=120
Temperature:	200 K		
	Calculated	Reported	
Volume	993.12(5)	993.12(5)	
Space group	P 32	P 32	
Hall group	P 32	P 32	
Moiety formula	C14 H17 N O3	C14 H17 N O3	
Sum formula	C14 H17 N O3	C14 H17 N O3	
Mr	247.29	247.28	
Dx, g cm-3	1.240	1.240	
Z	3	3	
Mu (mm-1)	0.711	0.711	
F000	396.0	396.0	
F000'	397.24		
h, k, lmax	17, 17, 6	17, 17, 6	
Nref	2416[1208]	2424	
Tmin, Tmax	0.787, 0.831	0.645, 0.753	
Tmin'	0.780		

Correction method= # Reported T Limits: Tmin=0.645 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 2.01/1.00 Theta(max)= 68.226

R(reflections)= 0.0368(2383) wR2(reflections)= 0.1032(2424)

S = 1.074 Npar= 177

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**

PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18)	6.85	Note
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.7	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.7	Ratio
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0051	Ang.

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	3	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	2	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	17%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
PLAT791_ALERT_4_G	Model has Chirality at C5 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C12 (Sohnke SpGr)	S	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	12	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	Info
PLAT996_ALERT_1_G	Non-Standard SHELXL LIST 4 Style FCF Supplied ..		! Check

0 **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
13 **ALERT level G** = General information/check it is not something unexpected

2 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
5 ALERT type 3 Indicator that the structure quality may be low
6 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.

