

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 = 0.0016 A	Wavelength=0.79272	
Cell:	a=14.2721(14)	b=19.479(2)	c=8.1900(9)
	alpha=90	beta=99.041(8)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	2248.6(4)	2248.6(4)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C14 H5 N3 O8, C14 H10	C14 H5 N3 O8, C14 H10	
Sum formula	C28 H15 N3 O8	C28 H15 N3 O8	
Mr	521.43	521.43	
Dx,g cm-3	1.540	1.540	
Z	4	4	
Mu (mm-1)	0.147	0.147	
F000	1072.0	1072.0	
F000'	1072.84		
h,k,lmax	18,25,10	18,25,10	
Nref	5152	5033	
Tmin,Tmax	0.974,0.996	0.966,0.987	
Tmin'	0.974		

Correction method= # Reported T Limits: Tmin=0.966 Tmax=0.987
AbsCorr = MULTI-SCAN

Data completeness= 0.977 Theta(max)= 30.950

R(reflections)= 0.0373(4596) wR2(reflections)= 0.0975(5033)

S = 1.023 Npar= 353

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

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full	value Low	.	0.977	Why?
PLAT369_ALERT_2_C	Long	C(sp2)-C(sp2) Bond	C5 - C6	.	1.54 Ang.
PLAT410_ALERT_2_C	Short	Intra H...H Contact	H1 ..H10	.	1.98 Ang.
			x,y,z =	1_555	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s)	Below Theta(Min).		6	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		89	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF		18	Note

● Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu				
	not performed for this radiation type.				
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka			0.79272	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O7 ..C5		2.92	Ang.
			x,y,l+z =	1_556	Check
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		24	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File	...		10	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		2.8	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			19	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **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

1 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
5 **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
2 **ALERT type 4** Improvement, methodology, query or suggestion
0 **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.

