

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) k-6

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: k-6

Bond precision:	C-C = 0.0040 A	Wavelength=0.71073	
Cell:	a=11.9094(14)	b=15.0748(12)	c=22.910(2)
	alpha=90	beta=100.961(9)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	4038.0(7)	4038.0(7)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C26 H22 N2 O3	2(C13 H11 N O1.5)	
Sum formula	C26 H22 N2 O3	C26 H22 N2 O3	
Mr	410.46	410.45	
Dx,g cm-3	1.350	1.350	
Z	8	8	
Mu (mm-1)	0.089	0.089	
F000	1728.0	1728.0	
F000'	1728.76		
h,k,lmax	14,17,27	14,17,27	
Nref	7114	7087	
Tmin,Tmax	0.988,0.989	0.730,1.000	
Tmin'	0.988		

Correction method= # Reported T Limits: Tmin=0.730 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 24.999

R(reflections)= 0.0647(5001) wR2(reflections)= 0.1568(7087)

S = 1.082 Npar= 571

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

PLAT420_ALERT_2_C	D-H Without Acceptor	N3	--H3	.	Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			14.414 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			2.210 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595			24 Report

Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ				Please Check
PLAT793_ALERT_4_G	Model has Chirality at C8	(Centro SPGR)			R Verify
PLAT793_ALERT_4_G	Model has Chirality at C9	(Centro SPGR)			S Verify
PLAT793_ALERT_4_G	Model has Chirality at C10	(Centro SPGR)			S Verify
PLAT793_ALERT_4_G	Model has Chirality at C11	(Centro SPGR)			S Verify
PLAT793_ALERT_4_G	Model has Chirality at C35	(Centro SPGR)			R Verify
PLAT793_ALERT_4_G	Model has Chirality at C36	(Centro SPGR)			S Verify
PLAT793_ALERT_4_G	Model has Chirality at C45	(Centro SPGR)			S Verify
PLAT793_ALERT_4_G	Model has Chirality at C46	(Centro SPGR)			S Verify
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still			42%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).				3 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				4 Info

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

1 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
5 ALERT type 3 Indicator that the structure quality may be low
8 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.

