

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) siv42

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: siv42

Bond precision:	C-C = 0.0050 A	Wavelength=0.71073	
Cell:	a=19.1157(8)	b=8.0014(3)	c=8.7287(4)
	alpha=90	beta=90	gamma=90
Temperature:	120 K		
	Calculated	Reported	
Volume	1335.08(10)	1335.08(10)	
Space group	P n m a	P n m a	
Hall group	-P 2ac 2n	-P 2ac 2n	
Moiety formula	C2 H9 B10 I3	C2 H9 B10 I3	
Sum formula	C2 H9 B10 I3	C2 H9 B10 I3	
Mr	521.89	521.89	
Dx, g cm ⁻³	2.596	2.596	
Z	4	4	
Mu (mm ⁻¹)	6.976	6.976	
F000	920.0	920.0	
F000'	914.59		
h, k, lmax	25, 10, 11	25, 10, 11	
Nref	1744	1739	
Tmin, Tmax	0.272, 0.377	0.229, 0.377	
Tmin'	0.207		

Correction method= # Reported T Limits: Tmin=0.229 Tmax=0.377
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 28.101

R(reflections)= 0.0224(1613)	wR2(reflections)= 0.0580(1739)
S = 1.143	Npar= 76

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 B

PLAT230_ALERT_2_B Hirshfeld Test Diff for I1 --I2_b . 7.5 s.u.



Alert level C

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.266 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report
PLAT977_ALERT_2_C Check Negative Difference Density on H6 . -0.49 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H8 . -0.54 eA-3



Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C1 Check
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C1 - C1_e . 1.68 Ang.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.29 Ratio
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 4 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

