

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) si357b

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: si357b

Bond precision:	C-C = 0.0023 A	Wavelength=0.71073	
Cell:	a=15.7323(17)	b=11.7003(13)	c=21.031(2)
	alpha=90	beta=107.188(1)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	3698.3(7)	3698.4(7)	
Space group	P 21/n	P 21/n	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C38 H98 K2 Si14, 2(C7 H8)	?	
Sum formula	C52 H114 K2 Si14	C26 H57 K Si7	
Mr	1210.89	605.44	
Dx,g cm-3	1.087	1.087	
Z	2	4	
Mu (mm-1)	0.384	0.384	
F000	1320.0	1320.0	
F000'	1323.27		
h,k,lmax	19,14,25	19,14,25	
Nref	6881	6854	
Tmin,Tmax	0.912,0.926	0.893,0.927	
Tmin'	0.891		

Correction method= # Reported T Limits: Tmin=0.893 Tmax=0.927
AbsCorr = EMPIRICAL

Data completeness= 0.996 Theta(max)= 25.500

R(reflections)= 0.0234(6366) wR2(reflections)= 0.0642(6854)

S = 1.049 Npar= 323

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**

PLAT220_ALERT_2_C	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for Si4	--C13 ..	5.4	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for Si5	--C16 ..	5.1	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for Si6	--C18 ..	5.1	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for Si7	--C10 ..	5.6	s.u.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	23	Report

● **Alert level G**

PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50	Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.26	Ratio
PLAT774_ALERT_1_G	Suspect X-Y Bond in CIF: K1 --K1 ..	4.43	Ang.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C7 H8	2	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	2	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	10	Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	2	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	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
10 **ALERT level G** = General information/check it is not something unexpected

3 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
3 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.

PLATON version of 09/11/2017; check.def file version of 08/11/2017

