

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) si301a

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: si301a

Bond precision: C-C = 0.0034 Å Wavelength=0.71073

Cell: a=11.3287(13) b=17.976(2) c=46.325(5)
 alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	9433.8(18)	9433.6(19)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C32 H76 Si11	?
Sum formula	C32 H76 Si11	C32 H76 Si11
Mr	769.92	769.91
Dx,g cm-3	1.084	1.084
Z	8	8
Mu (mm-1)	0.324	0.324
F000	3376.0	3376.0
F000'	3383.60	
h,k,lmax	13,21,55	13,21,55
Nref	8688	8683
Tmin,Tmax	0.968,0.990	0.694,0.746
Tmin'	0.968	

Correction method= # Reported T Limits: Tmin=0.694 Tmax=0.746
AbsCorr = EMPIRICAL

Data completeness= 0.999 Theta(max)= 25.408

R(reflections)= 0.0377(7366) wR2(reflections)= 0.0839(8683)

S = 1.099 Npar= 412

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**

PLAT213_ALERT_2_C	Atom C22	has ADP max/min Ratio	3.6	prolat
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range	6.0	Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 1 H	Uiso(max)/Uiso(min) Range	6.2	Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C21	Check
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of .		38	Ang**3
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		2.260	Check

● **Alert level G**

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	4	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	10.87	Why ?
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	18	Note
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	3	Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	9	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
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
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
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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.

