

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) si302a

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: si302a

Bond precision: C-C = 0.0037 A Wavelength=0.71073

Cell: a=11.5327(18) b=17.883(3) c=21.560(3)
 alpha=69.416(2) beta=85.458(2) gamma=76.379(2)

Temperature: 100 K

	Calculated	Reported
Volume	4045.5(11)	4045.5(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C48 H116 Si16), 5(C7 H8) ?	
Sum formula	C131 H272 Si32	C65.50 H136 Si16
Mr	2746.38	1373.17
Dx,g cm-3	1.127	1.127
Z	1	2
Mu (mm-1)	0.287	0.287
F000	1506.0	1506.0
F000'	1508.85	
h,k,lmax	14,22,27	14,22,27
Nref	16793	16153
Tmin,Tmax	0.944,0.972	0.692,0.746
Tmin'	0.944	

Correction method= # Reported T Limits: Tmin=0.692 Tmax=0.746
AbsCorr = EMPIRICAL

Data completeness= 0.962 Theta(max)= 26.500

R(reflections)= 0.0357(13586) wR2(reflections)= 0.0941(16153)

S = 1.037 Npar= 803

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	_diffn_measured_fraction_theta_full	value Low	0.972	Why?
PLAT220_ALERT_2_C	Non-Solvent Resd 1	C Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT223_ALERT_4_C	Solv./Anion Resd 4	H Ueq(max)/Ueq(min) Range	4.3	Ratio
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.8	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	3.1	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	406	Report
PLAT977_ALERT_2_C	Check Negative Difference Density on H17		-0.33	eA-3



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		7	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		7	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		0.50	Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.002	Degree
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		3	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		1	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C62	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C63	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C64	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C65	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C66	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C67	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C68	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H133	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H134	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H135	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H136	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H137	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H138	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H139	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H140	Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)		100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 4		7.50	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C55	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C69	Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		15	Check
PLAT793_ALERT_4_G	Model has Chirality at Si5	(Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at Si7	(Centro SPGR)	R	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		93	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	231	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		8	Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...		25	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		3	Info

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

- 2 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
8 **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
27 **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.

