

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: hannr05

Bond precision: C-C = 0.0050 A Wavelength=0.71073

Cell: a=11.936(3) b=13.097(3) c=13.758(3)
 alpha=80.165(5) beta=73.087(5) gamma=89.739(5)

Temperature: 100 K

	Calculated	Reported
Volume	2025.1(8)	2025.3(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C27 H63 Be K Si6	C27 H63 Be K Si6
Sum formula	C27 H63 Be K Si6	C27 H63 Be K Si6
Mr	604.42	604.42
Dx,g cm-3	0.991	0.991
Z	2	2
Mu (mm-1)	0.322	0.322
F000	664.0	664.0
F000'	665.48	
h,k,lmax	14,16,16	14,15,16
Nref	7746	7725
Tmin,Tmax	0.938,0.975	0.632,0.745
Tmin'	0.938	

Correction method= # Reported T Limits: Tmin=0.632 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 25.741

R(reflections)= 0.0588(4292) wR2(reflections)= 0.1326(7725)

S = 0.965 Npar= 370

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

PLAT049_ALERT_1_B Calculated Density less than 1.0 gcm-3 0.9912 Check

Author Response: This is correct.

Alert level C

PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 6.3 Ratio
PLAT245_ALERT_2_C U(iso) H12 Smaller than U(eq) C12 by ... 0.011 AngSq
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.005 Ang.
PLAT362_ALERT_2_C Short C(sp3)-C(sp2) Bond C2 - C3 .. 1.35 Ang.
PLAT362_ALERT_2_C Short C(sp3)-C(sp2) Bond C11 - C12 .. 1.35 Ang.

Alert level G

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.005 Degree
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 9 Note
PLAT343_ALERT_2_G Unusual sp3 Angle Range in Main Residue for C3 Check
PLAT343_ALERT_2_G Unusual sp3 Angle Range in Main Residue for C12 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.15 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 223 Check
K1 -C17 -H17A 1.555 1.555 1.555 44.00 Deg.
PLAT793_ALERT_4_G The Model has Chirality at C1 (Centro SPGR) R Verify
PLAT793_ALERT_4_G The Model has Chirality at C3 (Centro SPGR) S Verify
PLAT793_ALERT_4_G The Model has Chirality at C10 (Centro SPGR) R Verify
PLAT793_ALERT_4_G The Model has Chirality at C12 (Centro SPGR) S Verify
PLAT793_ALERT_4_G The Model has Chirality at C19 (Centro SPGR) R Verify
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 2 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
5 **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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 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.

PLATON version of 27/03/2017; check.def file version of 24/03/2017

