checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SSE_4

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: SSE_4

```
Bond precision:   C-C = 0.0066 A          Wavelength=1.54178

Cell:             a=56.6971(14)     b=56.6971(14)     c=12.7862(3)
                  alpha=90          beta=90           gamma=120
Temperature:      100 K
```

	Calculated	Reported
Volume	35595.4(19)	35595.5(19)
Space group	R -3	R -3
Hall group	-R 3	-R 3
Moiety formula	C47 H56 N6 O5 Si, C40 H43 N3 O3	C47 H56 N6 O5 Si, C40 H43 N3 O3
Sum formula	C87 H99 N9 O8 Si	C87 H99 N9 O8 Si
Mr	1426.84	1426.84
Dx,g cm-3	1.198	1.198
Z	18	18
Mu (mm-1)	0.751	0.751
F000	13716.0	13716.0
F000'	13758.72	
h,k,lmax	64,64,14	64,64,14
Nref	12173	12150
Tmin,Tmax	0.982,0.996	0.271,1.000
Tmin'	0.963	

```
Correction method= # Reported T Limits: Tmin=0.271 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 61.139

R(reflections)= 0.0683( 7490)                    wR2(reflections)=
                                                 0.1981( 12150)
S = 1.028                 Npar= 952
```

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 A

PLAT602_ALERT_2_A Solvent Accessible VOID(S) in Structure ..... ! Check

Author Response: Void investigated - no significant electron density found

---

Alert level B

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5680

Author Response: Diffraction intensity fell off sharply with increasing resolution. Max data resolution was cut to F^2^/\sF^2^ > 2 during data processing.

Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.3 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.4 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si01 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C100 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00657 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 5.723 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.568 26 Report

---

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 36.38 Why ?
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 183 Note
PLAT793_ALERT_4_G Model has Chirality at C034 (Centro SPGR) S Verify
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 35% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.9 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

---

1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **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
  8 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
```

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 12/09/2022; check.def file version of 09/08/2022

Datablock SSE_4 - ellipsoid plot