checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3

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: 3

Bond precision: C-C = 0.0300 A Wavelength=0.71073

Cell: a=18.5833(3) b=18.5833(3) c=27.7469(8)
alpha=90 beta=90 gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	9582.1(4)	9582.1(5)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C36 H84 I N2 Si4 U [+ solvent]	C36 H84 I N2 Si4 U
Sum formula	C36 H84 I N2 Si4 U [+ solvent]	C36 H84 I N2 Si4 U
Mr	1022.34	1022.34
Dx,g cm-3	1.417	1.417
Z	8	8
Mu (mm-1)	4.156	4.156
F000	4120.0	4120.0
F000’	4042.90	
h,k,lmax	22,22,33	22,22,33
Nref	4382	4372
Tmin,Tmax	0.593,0.753	0.846,1.000
Tmin’	0.558	

Correction method= # Reported T Limits: Tmin=0.846 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.998 Theta(max)= 25.338

R(reflections)= 0.0880(3542) wR2(reflections)= 0.2119(4372)

S = 1.154 Npar= 320

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

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.03 Ang.

Author Response: Low C-C bond precision is the result of unresolved modulation in the diffraction data which presents as two versions of the entire molecule, pointing in oposite directions along the U-I axis. Typically this can be resolved to some degree by modelling the entire structure over two positions and refining them competetively with strong restraints on the second (low occupancy) component; however in this instance the large amount of disorder about Si2 made modelling the modulation in this way unsatisfactory and did not result in a better model. This modulation also results in a larger than normal residual peak which we have attributed to the second U component.

Alert level C

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of U1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si1 Check
PLAT412_ALERT_2_C Short Intra XH3 .. XHn H8B ..H9BB .. 1.85 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 11.913 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.583 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 9 Note
PLAT977_ALERT_2_C Check Negative Difference Density on H13A -0.31 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 24 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 34 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 922.90 Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 4 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) U1 --I1 . 13.1 s.u.
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 50% Note
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 127 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 6 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 511 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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0 **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
15 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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 10 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
  6 ALERT type 4 Improvement, methodology, query or suggestion
  1 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.

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

Datablock 3 - ellipsoid plot