

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 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: 4

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Bond precision:	C-C = 0.0073 A	Wavelength=0.71073
Cell:	a=10.8290(5)      b=12.4282(5)      c=12.9502(5)	
	alpha=90      beta=94.783(4)      gamma=90	
Temperature:	150 K	
	Calculated	Reported
Volume	1736.83(13)	1736.85(13)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	C26 H58 I2 N O2 Si2 U	C26 H58 I2 N O2 Si2 U
Sum formula	C26 H58 I2 N O2 Si2 U	C26 H58 I2 N O2 Si2 U
Mr	964.74	964.74
Dx,g cm-3	1.845	1.845
Z	2	2
Mu (mm-1)	6.541	6.541
F000	926.0	926.0
F000'	905.58	
h,k,lmax	13,14,15	13,14,15
Nref	3183	3182
Tmin,Tmax	0.732,0.780	0.876,0.962
Tmin'	0.639	

Correction method= # Reported T Limits: Tmin=0.876 Tmax=0.962  
AbsCorr = GAUSSIAN

Data completeness= 1.000      Theta(max)= 25.348

R(reflections)= 0.0319( 2654)      wR2(reflections)= 0.0518( 3182)

S = 1.004      Npar= 171

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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.

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## ● Alert level C

PLAT978\_ALERT\_2\_C Number C-C Bonds with Positive Residual Density. 0 Info

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## ● Alert level G

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 4 Note  
PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 6 Report  
PLAT176\_ALERT\_4\_G The CIF-Embedded .res File Contains SADI Records 2 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  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 1 ) 6% Note  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 67 Note  
PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
1 **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  
3 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 ALERT type 3 Indicator that the structure quality may be low  
3 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.

Datablock 4 - ellipsoid plot

