

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 5

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: 5

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Bond precision:	C-C = 0.0190 Å	Wavelength=0.71073
Cell:	a=23.6408(16)	b=10.9612(13)      c=27.4164(15)
	alpha=90	beta=97.384(6)      gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	7045.5(10)	7045.6(10)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C48 H118 Cl2 N4 Si8 U2	C48 H118 Cl2 N4 Si8 U2
Sum formula	C48 H118 Cl2 N4 Si8 U2	C48 H118 Cl2 N4 Si8 U2
Mr	1523.14	1523.14
Dx,g cm-3	1.436	1.436
Z	4	4
Mu (mm-1)	4.834	4.834
F000	3056.0	3056.0
F000'	2983.64	
h,k,lmax	28,13,33	28,13,33
Nref	6468	6459
Tmin,Tmax	0.617,0.695	0.913,0.981
Tmin'	0.283	

Correction method= # Reported T Limits: Tmin=0.913 Tmax=0.981  
AbsCorr = GAUSSIAN

Data completeness= 0.999      Theta(max)= 25.350

R(reflections)= 0.0609( 3184)      wR2(reflections)= 0.1580( 6459)

S = 1.006      Npar= 484

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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

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..	49%	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.019	Ang.
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	10	Note
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.93A From U1	-1.59	eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on U1	1.47	eA-3
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	21	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	50	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	7.37	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
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	56%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	30	Note
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C21B --C23B	1.74	Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #	73	Check
	U1 -C1A -H1AC 1.555 1.555 1.555	35.20	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #	249	Check
	U1 -C19B -H19D 1.555 1.555 1.555	28.70	Deg.
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	737	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	1	Note
PLAT955_ALERT_1_G	Reported (CIF) and Actual (FCF) Lmax Differ by .	1	Units

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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  
6 **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

1 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  
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.

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

