# 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: 3**

Bond precision:	C-C = 0.0066 A Wavelengt		Navelength=1	1.54184		
Cell:	a=13.3675(2) alpha=90 100 K		3) 19(17)			
Temperature:	100 K					
	Calculated		Reported			
Volume	4867.75(15)		4867.74(15)	)		
Space group	P 21/c		P 1 21/c 1			
	-P 2ybc		-P 2ybc			
Moiety formula	C32 H68 Cl4 Mg O H8 O	4 Si4 U, C4	C32 H68 Cl H8 O	4 Mg O4 Si4 U, C4		
Sum formula	C36 H76 C14 Mg O	5 Si4 U	C36 H76 Cl.	4 Mg O5 Si4 U		
Mr	1105.47		1105.46			
Dx,g cm-3	1.508		1.508			
Z	4		4			
Mu (mm-1)	12.758		12.758			
F000	2240.0		2240.0			
F000′	2237.55					
h,k,lmax			16,18,28			
	9247		9215			
	0.264,0.448		0.217,0.58	5		
Tmin'	0.071					
Correction method= # Reported T Limits: Tmin=0.217 Tmax=0.585 AbsCorr = ANALYTICAL						
Data completeness= 0.997 Theta(max)= 70.068						
R(reflections)=		wR2(reflections) 0.0760( 9215)				
S = 1.038	Npar=	502		,		

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 C

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.5 Ratio

#### Alert level G

ATELC LEVEL G	
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	12 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms	2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records	6 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records	2 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) U1Cl1 .	9.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) U1Cl2 .	7.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) U1Cl3 .	8.8 s.u.
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1 )	4% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2 )	20% Note
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O5 .	101.7 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels	4 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints	18 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	2.8 Low

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 13 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 3 ALERT type 3 Indicator that the structure quality may be low 4 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 18/05/2022; check.def file version of 17/05/2022

Datablock 3 - ellipsoid plot

