

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) RGFTS03602\_sq

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: RGFTS03602\_sq

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Bond precision:    C-C = 0.0078 Å                      Wavelength=0.71073

Cell:                      a=20.5866(10)              b=20.5866(10)              c=20.5866(10)  
                                    alpha=90                      beta=90                      gamma=90

Temperature:              199 K

	Calculated	Reported
Volume	8724.8(13)	8724.8(13)
Space group	P a -3	P a -3
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C39 H57 Cl N6 U [+ solvent]	C39 H57 Cl N6 U
Sum formula	C39 H57 Cl N6 U [+ solvent]	C39 H57 Cl N6 U
Mr	883.39	883.38
Dx, g cm <sup>-3</sup>	1.345	1.345
Z	8	8
Mu (mm <sup>-1</sup> )	3.813	3.813
F000	3536.0	3536.0
F000'	3461.23	
h, k, lmax	24, 24, 24	24, 24, 24
Nref	2717	2714
Tmin, Tmax	0.599, 0.657	0.579, 0.745
Tmin'	0.451	

Correction method= # Reported T Limits: Tmin=0.579 Tmax=0.745  
AbsCorr = MULTI-SCAN

Data completeness= 0.999                      Theta(max)= 25.478

R(reflections)= 0.0360( 1842)

wR2(reflections)=  
0.0822( 2714)

S = 1.035

Npar= 146

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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**

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	4.530	Check
PLAT974_ALERT_2_C	Check Calcd Negative Resid. Density on U1	-1.11	eA-3

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● **Alert level G**

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	10.39	Why ?
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	259	A**3
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.14	Ratio
PLAT794_ALERT_5_G	Tentative Bond Valency for U1 (IV) .	3.81	Info
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed		! Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min). 1 1 1, 0 0 2,	2	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF .... 0 0 2,	1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File 1 1 3, 0 0 2,	2	Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....		Please Check
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	51.0	Degree
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....	2.51	Note
	Predicted wR2: Based on SigI**2 3.28 or SHELX Weight	8.17	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	Info

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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  
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
14 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
5 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  
4 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 13/12/2023; check.def file version of 13/12/2023**

