

# 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: dq0090\_cc

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Bond precision:    C-C = 0.0123 Å                      Wavelength=0.71073

Cell:                      a=11.0688(9)              b=29.295(3)              c=8.7573(7)  
                                alpha=90                      beta=102.609(1)              gamma=90

Temperature:              100 K

	Calculated	Reported
Volume	2771.2(4)	2771.2(4)
Space group	C c	C c
Hall group	C -2yc	?
Moiety formula	C24 H38 Br2 K O U	?
Sum formula	C24 H38 Br2 K O U	C24 H38 Br2 K O U
Mr	779.47	779.49
Dx,g cm-3	1.868	1.868
Z	4	4
Mu (mm-1)	8.903	8.903
F000	1484.0	1484.0
F000'	1445.09	
h,k,lmax	17,46,13	17,46,13
Nref	11567[ 5795]	11401
Tmin,Tmax	0.136,0.411	0.206,0.470
Tmin'	0.086	

Correction method= # Reported T Limits: Tmin=0.206 Tmax=0.470  
AbsCorr = MULTI-SCAN

Data completeness= 1.97/0.99                      Theta(max)= 34.290

R(reflections)= 0.0483( 10755)              wR2(reflections)= 0.1308( 11401)

S = 1.152                      Npar= 273

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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**

PLAT213_ALERT_2_C	Atom C16	has ADP max/min Ratio .....	3.5	prolat
PLAT213_ALERT_2_C	Atom C18	has ADP max/min Ratio .....	3.4	prolat
PLAT220_ALERT_2_C	Large Non-Solvent C	Ueq(max)/Ueq(min) Range	5.4	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C12 -- C17 ..		5.8	s.u.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C24	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....		0.01235	Ang.

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● **Alert level G**

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		1	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		1	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF			Please Do !
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as			mixed Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) U1 -- Br1 ..		7.0	s.u.
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .		1.17	Ratio
PLAT774_ALERT_1_G	Suspect X-Y Bond in CIF: K1 -- K1 ..		4.46	Ang.
PLAT774_ALERT_1_G	Suspect X-Y Bond in CIF: K1 -- K1 ..		4.46	Ang.
PLAT774_ALERT_1_G	Suspect X-Y Bond in CIF: K1 -- U1 ..		4.56	Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #		176	Check
	O1 -C24 -K1 1.555 1.555 1.555		41.50	Deg.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		8	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL		2014	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  
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
12 **ALERT level G** = General information/check it is not something unexpected

4 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  
2 ALERT type 3 Indicator that the structure quality may be low  
3 ALERT type 4 Improvement, methodology, query or suggestion  
2 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*, 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.

