

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) BS9\_0M\_A

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: BS9\_0M\_A

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Bond precision:	C-C = 0.0036 A	Wavelength=0.71073
Cell:	a=11.975(2)	b=6.8162(11)      c=18.711(3)
	alpha=90	beta=98.345(4)      gamma=90
Temperature:	294 K	
	Calculated	Reported
Volume	1511.1(4)	1511.2(4)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	2(C17 H14 F N3 O2), H2 O	2(C17 H14 F N3 O2), H2 O
Sum formula	C34 H30 F2 N6 O5	C34 H30 F2 N6 O5
Mr	640.64	640.64
Dx,g cm-3	1.408	1.408
Z	2	2
Mu (mm-1)	0.105	0.105
F000	668.0	668.0
F000'	668.34	
h,k,lmax	16,9,25	15,9,24
Nref	3785	3739
Tmin,Tmax	0.958,0.977	0.930,0.960
Tmin'	0.958	

Correction method= # Reported T Limits: Tmin=0.930 Tmax=0.960  
AbsCorr = MULTI-SCAN

Data completeness= 0.988      Theta(max)= 28.389

R(reflections)= 0.0649( 2632)      wR2(reflections)= 0.1637( 3739)

S = 1.097      Npar= 224

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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 .....	6.743	Check
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance .....	2.389	Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	14	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF ....	5	Note
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....	1	Check

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● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3	Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of *O1W is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H1W is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H2W is Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)..	100 %	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms ( 1.50) in Resd. #	2	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	2	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min)	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	30	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	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  
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
11 **ALERT level G** = General information/check it is not something unexpected

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
2 ALERT type 2 Indicator that the structure model may be wrong or deficient  
7 ALERT type 3 Indicator that the structure quality may be low  
7 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.

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**PLATON version of 24/11/2016; check.def file version of 23/11/2016**

