

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) bmk1918

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: bmk1918

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Bond precision:    C-C = 0.0056 A

Wavelength=0.71073

Cell:                a=7.7344(6)                b=18.2778(12)                c=19.4909(12)  
                      alpha=116.181(6)        beta=96.410(6)        gamma=92.091(6)  
Temperature:        293 K

	Calculated	Reported
Volume	2445.9(3)	2445.9(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C27 H19 Cl F2 N6 S	?
Sum formula	C27 H19 Cl F2 N6 S	C27 H19 Cl F2 N6 S
Mr	532.99	532.99
Dx,g cm-3	1.447	1.447
Z	4	4
Mu (mm-1)	0.287	0.287
F000	1096.0	1096.0
F000'	1097.51	
h,k,lmax	10,25,27	10,24,26
Nref	13849	11546
Tmin,Tmax	0.978,0.993	0.791,1.000
Tmin'	0.925	

Correction method= # Reported T Limits: Tmin=0.791 Tmax=1.000  
AbsCorr = GAUSSIAN

Data completeness= 0.834

Theta(max)= 29.664

R(reflections)= 0.0652( 4785)

wR2(reflections)= 0.1666( 11546)

S = 1.014

Npar= 670

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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 ..	41%	Check
PLAT334_ALERT_2_C	Small Aver. Benzene C-C Dist C22 -C27	1.37	Ang.
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00556	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H17 ..N10	2.67	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H17 ..N11	2.67	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	16.004	Check

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● **Alert level G**

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.006	Degree
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .....	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature .....	293	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Cl2 ..F1	2.99	Ang.
	1-x,1-y,2-z =	2_667	Check
PLAT793_ALERT_4_G	Model has Chirality at C10 (Centro SPGR)		R Verify
PLAT793_ALERT_4_G	Model has Chirality at C37 (Centro SPGR)		S Verify
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	2267	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	2.0	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	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  
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
10 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 ALERT type 2 Indicator that the structure model may be wrong or deficient  
4 ALERT type 3 Indicator that the structure quality may be low  
5 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.

