

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1494\_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: 1494\_0m\_a

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Bond precision:    C-C = 0.0023 A

Wavelength=0.71073

Cell:                    a=7.591(4)                    b=10.496(4)                    c=10.791(5)  
                          alpha=86.56(3)                    beta=85.43(2)                    gamma=70.61(3)  
Temperature:            293 K

	Calculated	Reported
Volume	807.9(7)	808.0(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C10 H12 B2 F4 O4 S, 0.5(C2 H4 Cl2)	C10 H12 B2 F4 O4 S, C H2 Cl
Sum formula	C11 H14 B2 Cl F4 O4 S	C11 H14 B2 Cl F4 O4 S
Mr	375.35	375.35
Dx,g cm-3	1.543	1.543
Z	2	2
Mu (mm-1)	0.419	0.419
F000	382.0	382.0
F000'	382.81	
h,k,lmax	14,19,20	14,19,20
Nref	10860	10786
Tmin,Tmax	0.713,0.849	0.722,0.854
Tmin'	0.699	

Correction method= # Reported T Limits: Tmin=0.722 Tmax=0.854

AbsCorr = MULTI-SCAN

Data completeness= 0.993

Theta(max)= 41.330

R(reflections)= 0.0669( 6303)

wR2(reflections)= 0.2078( 10786)

S = 1.021

Npar= 212

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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.



#### Alert level B

CRYSS02\_ALERT\_3\_B The value of \_exptl\_crystal\_size\_mid is > 0.8  
Mid crystal size given = 0.810



#### Alert level C

ABSTY02\_ALERT\_1\_C An \_exptl\_absorpt\_correction\_type has been given without  
a literature citation. This should be contained in the  
\_exptl\_absorpt\_process\_details field.

Absorption correction given as multi-scan

PLAT242_ALERT_2_C Low	'MainMol' Ueq as Compared to Neighbors of	B1	Check
PLAT242_ALERT_2_C Low	'MainMol' Ueq as Compared to Neighbors of	B2	Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including	C11	0.103	Check
PLAT336_ALERT_2_C Long Bond Distance for	..... C11 -C11	1.858	Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond	C11 - C11_a	1.38	Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	.....	11.661	Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	.....	2.573	Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=	0.600	5	Report
PLAT977_ALERT_2_C Check Negative Difference Density on H1C		-0.38	eA-3



#### Alert level G

PLAT012_ALERT_1_G No	_shelx_res_checksum Found in CIF	.....	Please	Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ			Please	Check
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size	....	0.83	mm	
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large		0.10	Report	
PLAT199_ALERT_1_G Reported _cell_measurement_temperature	..... (K)	293	Check	
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature	..... (K)	293	Check	
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).		3	Note	
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=	0.600	64	Note	
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File	...	3	Note	
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		4	Info	

0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

10 **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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

9 ALERT type 2 Indicator that the structure model may be wrong or deficient

5 ALERT type 3 Indicator that the structure quality may be low

2 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.

