

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1491_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: 1491_0m_a

Bond precision: C-C = 0.0028 Å Wavelength=0.71073

Cell: a=11.371(9) b=12.765(11) c=11.993(9)
 alpha=90 beta=116.24(3) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	1561(2)	1561(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C11 H14 B2 F4 O5 S	C11 H14 B2 F4 O5 S
Sum formula	C11 H14 B2 F4 O5 S	C11 H14 B2 F4 O5 S
Mr	355.90	355.90
Dx,g cm-3	1.514	1.514
Z	4	4
Mu (mm-1)	0.269	0.269
F000	728.0	728.0
F000'	729.07	
h,k,lmax	15,17,16	15,17,16
Nref	4116	4100
Tmin,Tmax	0.905,0.930	0.902,0.931
Tmin'	0.900	

Correction method= # Reported T Limits: Tmin=0.902 Tmax=0.931
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 28.900

R(reflections)= 0.0404(3356) wR2(reflections)= 0.1217(4100)

S = 1.052 Npar= 212

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 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

● Alert level G

PLAT012_ALERT_1_G	No	_shelx_res_checksum Found in CIF		Please Check
PLAT066_ALERT_1_G		Predicted and Reported Tmin&Tmax Range Identical		? Check
PLAT199_ALERT_1_G		Reported _cell_measurement_temperature	(K)	293 Check
PLAT200_ALERT_1_G		Reported _diffrn_ambient_temperature	(K)	293 Check
PLAT432_ALERT_2_G		Short Inter X...Y Contact F1 ..C9		2.91 Ang.
		1-x,1-y,1-z =	3_666	Check
PLAT910_ALERT_3_G		Missing # of FCF Reflection(s) Below Theta(Min).		4 Note
PLAT912_ALERT_4_G		Missing # of FCF Reflections Above STh/L= 0.600		12 Note
PLAT913_ALERT_3_G		Missing # of Very Strong Reflections in FCF		1 Note
PLAT978_ALERT_2_G		Number C-C Bonds with Positive Residual Density.		8 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected

- 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
1 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.

