

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) xsm_auto

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: xsm_auto

Bond precision:	C-C = 0.0028 A	Wavelength=1.54184
Cell:	a=7.64930 (7)	b=11.76455 (11) c=15.33719 (15)
	alpha=90	beta=90 gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	1380.20 (2)	1380.20 (2)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C12 H24 B F2 N O	C12 H24 B F2 N O
Sum formula	C12 H24 B F2 N O	C12 H24 B F2 N O
Mr	247.13	247.13
Dx, g cm ⁻³	1.189	1.189
Z	4	4
Mu (mm ⁻¹)	0.756	0.756
F000	536.0	536.0
F000'	537.73	
h, k, lmax	9, 14, 18	9, 14, 18
Nref	2724 [1583]	2689
Tmin, Tmax	0.947, 0.970	0.655, 1.000
Tmin'	0.941	

Correction method= # Reported T Limits: Tmin=0.655 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.70/0.99 Theta(max)= 72.028

R(reflections)= 0.0357 (2656)	wR2(reflections)=
S = 1.095	0.0969 (2689)
Npar= 161	

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

PLAT031_ALERT_4_C	Refined Extinction Parameter Within Range of ...	2.700 Sigma
PLAT410_ALERT_2_C	Short Intra H...H Contact H11 ..H15A .	1.98 Ang.
	x,y,z =	1_555 Check
PLAT412_ALERT_2_C	Short Intra XH3 .. XHn H11 ..H17A .	1.85 Ang.
	x,y,z =	1_555 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	3 Report



Alert level G

PLAT142_ALERT_4_G	s.u. on b - Axis Small or Missing	0.00011 Ang.
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing	0.00015 Ang.
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	9 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.	7 Info

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

0 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
2 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

start Validation Reply Form

_vrf_PLAT031_xsm_auto

;

PROBLEM: Refined Extinction Parameter Within Range of ... 2.700 Sigma

RESPONSE: ...

;

_vrf_PLAT410_xsm_auto

;

PROBLEM: Short Intra H...H Contact H11 ..H15A . 1.98 Ang.

RESPONSE: ...

;

_vrf_PLAT412_xsm_auto

;

PROBLEM: Short Intra XH3 .. XHn H11 ..H17A . 1.85 Ang.

RESPONSE: ...

;

_vrf_PLAT911_xsm_auto

```
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.600      3 Report
RESPONSE: ...
;
# end Validation Reply Form
```

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.

PLATON version of 10/05/2023; check.def file version of 10/05/2023

