checkCIF/PLATON report

Structure factors have been supplied for datablock(s) FO6304, FO6401

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: FO6304

Bond precision: C-C = 0.0031 A Wavelength=0.71073

Cell: a=14.4922(3) b=14.2458(2) c=15.9319(3)
alpha=90 beta=91.960(1) gamma=90
Temperature: 133 K

	Calculated	Reported
Volume	3287.26(10)	3287.26(10)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C19 H19 B F2 N2 O	C19 H19 B F2 N2 O
Sum formula	C19 H19 B F2 N2 O	C19 H19 B F2 N2 O
Mr	340.17	340.17
Dx,g cm-3	1.375	1.375
Z	8	8
Mu (mm-1)	0.100	0.100
F000	1424.0	1424.0
F000’	1424.73	
h,k,lmax	18,18,20	18,18,20
Nref	7537	7523
Tmin,Tmax	0.988,0.991	0.703,0.746
Tmin’	0.988	

Correction method= # Reported T Limits: Tmin=0.703 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 27.480

R(reflections)= 0.0600(5331) wR2(reflections)= 0.1222(7523)

S = 1.094 Npar= 467

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

```
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     11.775 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.334 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          3 Report
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Alert level G

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PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          6 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2018 Note
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         9 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
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 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
3 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: FO6401

Bond precision: C-C = 0.0089 A Wavelength=0.71073

Cell: a=21.8579(4) b=10.5698(2) c=18.2672(4)
alpha=90 beta=112.645(1) gamma=90
Temperature: 133 K

	Calculated	Reported
Volume	3894.98(14)	3894.98(13)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C19 H17 B F2 I2 N2 O	C19 H17 B F2 I2 N2 O
Sum formula	C19 H17 B F2 I2 N2 O	C19 H17 B F2 I2 N2 O
Mr	591.96	591.96
Dx,g cm-3	2.019	2.019
Z	8	8
Mu (mm-1)	3.260	3.260
F000	2256.0	2256.0
F000’	2249.34	
h,k,lmax	28,13,23	28,13,23
Nref	8931	8873
Tmin,Tmax	0.758,0.775	0.628,0.746
Tmin’	0.743	

Correction method= # Reported T Limits: Tmin=0.628 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 27.480

R(reflections)= 0.0554(6854) wR2(reflections)= 0.1062(8873)

S = 1.132 Npar= 503

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

PLAT213_ALERT_2_B Atom C8B has ADP max/min Ratio ..... 4.4 oblate

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Alert level C

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.
bordeauxe
PLAT213_ALERT_2_C Atom C17B has ADP max/min Ratio ..... 3.2 oblate
PLAT245_ALERT_2_C U(iso) H1OA Smaller than U(eq) O1A by 0.011 Ang**2
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00895 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 8.007 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 26 Report
PLAT977_ALERT_2_C Check Negative Difference Density on H10A -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H11B -0.45 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H13D -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H16B -0.31 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

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Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 30.51 Why ?
PLAT432_ALERT_2_G Short Inter X...Y Contact F1A ..C6B 2.94 Ang.
1-x,-1/2+y,3/2-z = 2_646 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 2 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2018 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 36 Note

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checkCIF publication errors

Alert level G

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PUBL017_ALERT_1_G The _publ_section_references section is missing or
           empty.
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   0 ALERT level A = Data missing that is essential or data in wrong format
   1 ALERT level G = General alerts. Data that may be required is missing
```

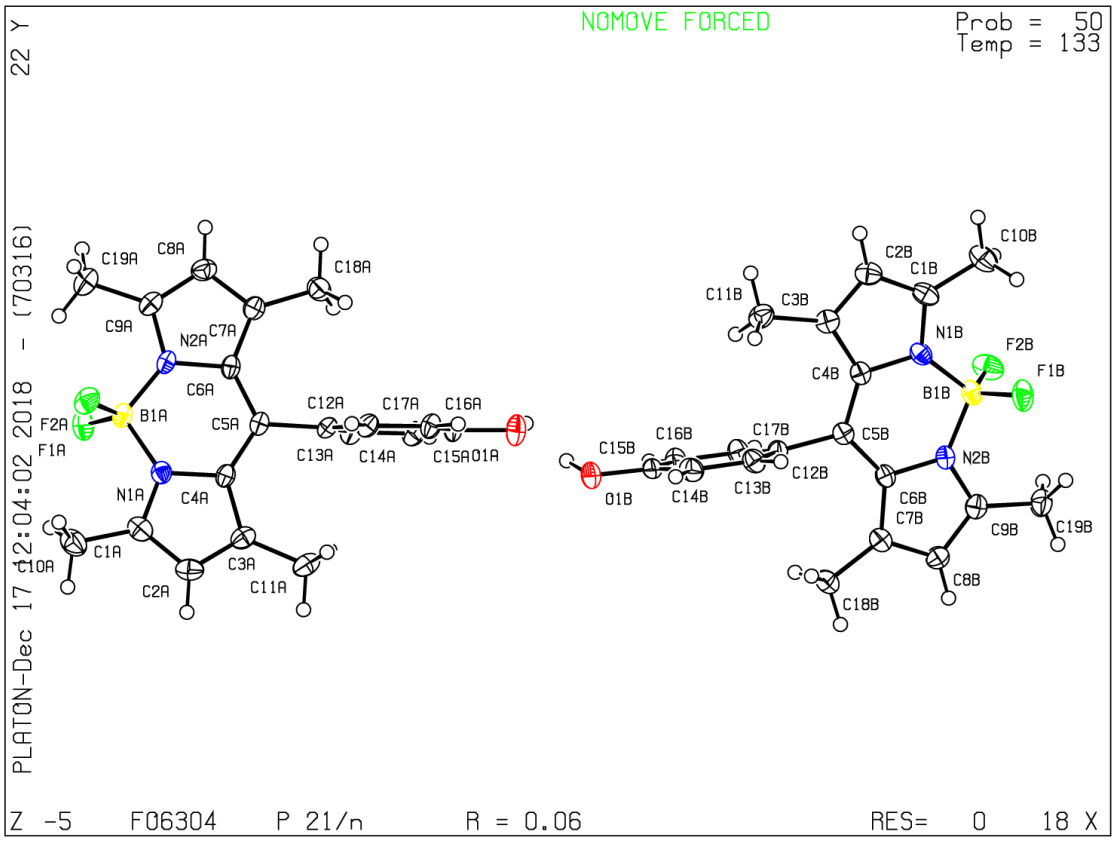
Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 13/12/2018; check.def file version of 11/12/2018

Datablock FO6304 - ellipsoid plot



Datablock FO6401 - ellipsoid plot