checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: i13541y

Bond precision: C-C = 0.0038 A Wavelength=0.71073

Cell: a=8.8382(6) b=18.6613(12) c=12.5173(9)
alpha=90 beta=106.714(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1977.3(2)	1977.3(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C18 H28 N3, B F4	C18 H28 N3, B F4
Sum formula	C18 H28 B F4 N3	C18 H28 B F4 N3
Mr	373.24	373.24
Dx,g cm-3	1.254	1.254
Z	4	4
Mu (mm-1)	0.100	0.100
F000	792.0	792.0
F000'	792.44	
h,k,lmax	11,24,16	11,24,16
Nref	4533	4535
Tmin,Tmax	0.981,0.988	0.907,0.970
Tmin'	0.980	

Correction method= MULTI-SCAN

Data completeness= 1.000 Theta(max)= 27.480

R(reflections)= 0.0696(2670) wR2(reflections)= 0.1843(4535)

S = 1.043 Npar= 249

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

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -0.788
Test value = -0.675
DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.
DIFMX01_ALERT_2_C The maximum difference density is > 0.1*ZMAX*0.75

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           _refine_diff_density_max given =      0.831
           Test value =      0.675
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       0.83 eA-3
PLAT098_ALERT_2_C Large Reported Min.  (Negative) Residual Density      -0.79 eA-3
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of          B1
PLAT420_ALERT_2_C D-H Without Acceptor       N3     -   H3     ...          ?
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Alert level G

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PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c   .......      P21/n
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
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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
8 **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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 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*, 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 19/04/2012; check.def file version of 14/04/2012

Datablock i13541y - ellipsoid plot