checkCIF/PLATON report

Structure factors have been supplied for datablock(s) jb210121_1_1_twin1_hklf4

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: jb210121_1_1_twin1_hklf4

```
Bond precision:  C-C = 0.0043 A          Wavelength=1.54184

Cell:          a=7.6684(2)       b=9.2792(2)      c=18.6002(6)
               alpha=85.355(2)   beta=87.229(2)   gamma=84.797(2)
Temperature:   100 K

                Calculated                Reported
Volume          1312.62(6)                1312.62(6)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  C13 H13 B F3 N O3         C13 H13 B F3 N O3
Sum formula     C13 H13 B F3 N O3         C13 H13 B F3 N O3
Mr              299.05                    299.05
Dx,g cm-3       1.513                     1.513
Z               4                         4
Mu (mm-1)       1.157                     1.157
F000            616.0                     616.0
F000'           618.48
h,k,lmax        9,11,23                   9,11,23
Nref            5726                      6292
Tmin,Tmax       0.858,0.953               0.773,1.000
Tmin'           0.843

Correction method= # Reported T Limits: Tmin=0.773 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 1.099          Theta(max)= 79.873

R(reflections)= 0.0590( 5511)     wR2(reflections)= 0.2352( 6292)

S = 1.137                  Npar= 388
```

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

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O1A      ..O1A      .       2.84 Ang.
                                                -x,2-y,-z  =      2_575 Check
```

Alert level C

```
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00427 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         85 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .         30 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .      34.96 Check
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          4 Note
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.14 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.002 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          2 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        262 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.2 Low
```

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

   1 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
   6 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

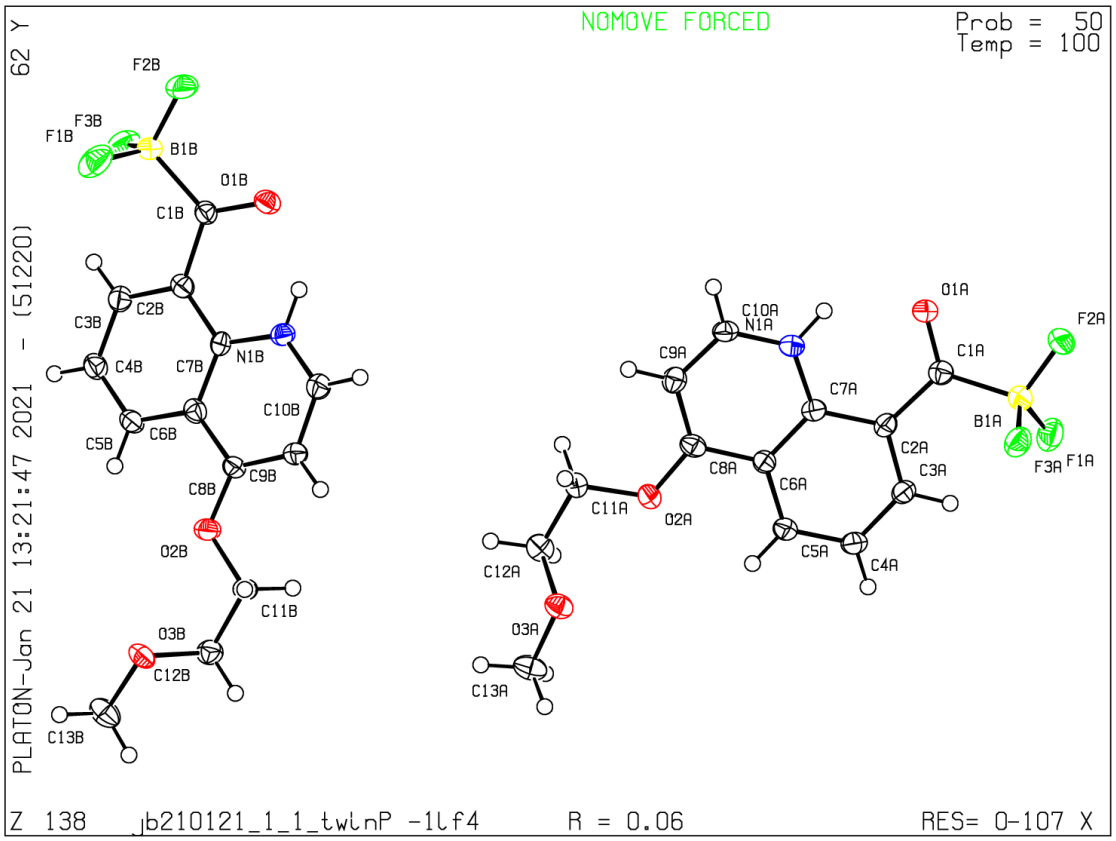
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.

PLATON version of 05/12/2020; check.def file version of 05/12/2020

Datablock jb210121_1_1_twin1_hklf4 - ellipsoid plot