checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: mo_gk_phbno3_0m

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Bond precision:   C-C = 0.0040 A          Wavelength=0.71073

Cell:             a=10.1256(5)     b=16.8204(13)      c=18.9207(16)
                  alpha=90         beta=98.178(2)     gamma=90
Temperature:      160 K

                 Calculated                Reported
Volume           3189.7(4)                 3189.7(4)
Space group      P 21/c                    P 1 21/c 1
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C33 H43 B N4 O6           C33 H43 B N4 O6
Sum formula      C33 H43 B N4 O6           C33 H43 B N4 O6
Mr               602.52                    602.52
Dx,g cm-3        1.255                     1.255
Z                4                         4
Mu (mm-1)        0.086                     0.086
F000             1288.0                    1288.0
F000'            1288.57
h,k,lmax         14,23,26                  13,21,26
Nref             8946                      7552
Tmin,Tmax        0.988,0.993               0.683,0.746
Tmin'            0.984

Correction method= # Reported T Limits: Tmin=0.683 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.844           Theta(max)= 29.578

R(reflections)= 0.0693( 3960)                wR2(reflections)=
                                             0.2175( 7552)
S = 0.995                  Npar= 405
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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

PLAT230_ALERT_2_B Hirshfeld Test Diff for O5 --N4 . 7.5 s.u.

Author Response: All atoms are assigned appropriately and it is caused by the vibration of nitro group

PLAT230_ALERT_2_B Hirshfeld Test Diff for O5 --B1 . 8.0 s.u.

Author Response: All atoms are assigned appropriately and it is caused by the vibration of nitro group

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Alert level C

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -0.760
Test value = -0.600
DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density -0.76 eA-3
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 3.8 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for O6 --N3 . 6.9 s.u.

Author Response: All atoms are assigned appropriately and it is caused by the vibration of nitro group

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N4 Check

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Alert level G

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 2.9 Low
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 2 Units

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
0 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* 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 18/05/2022; check.def file version of 17/05/2022

Datablock mo_gk_phbno3_0m - ellipsoid plot