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: faces-xstr1656_filtered

```
Bond precision:    C-C = 0.0016 A              Wavelength=1.54184

Cell:              a=6.81856(4)     b=18.79523(11)      c=32.85532(19)
                   alpha=90         beta=90             gamma=90
Temperature:       150 K

                   Calculated                 Reported
Volume             4210.62(4)                 4210.62(4)
Space group        P b c a                    P b c a
Hall group         -P 2ac 2ab                 -P 2ac 2ab
Moiety formula     C23 H21 B3 N2 O3           C23 H21 B3 N2 O3
Sum formula        C23 H21 B3 N2 O3           C23 H21 B3 N2 O3
Mr                 405.85                     405.85
Dx,g cm-3          1.280                      1.280
Z                  8                          8
Mu (mm-1)          0.658                      0.657
F000               1696.0                     1696.0
F000'              1700.94
h,k,lmax           8,22,39                    8,22,39
Nref               3714                       3713
Tmin,Tmax          0.910,0.974                0.883,0.975
Tmin'              0.860

Correction method= # Reported T Limits: Tmin=0.883 Tmax=0.975
AbsCorr = ANALYTICAL

Data completeness= 1.000          Theta(max)= 66.590

R(reflections)= 0.0306( 3408)                      wR2(reflections)=
                                                   0.0824( 3713)
S = 1.036                 Npar= 286
```

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**

PLAT420_ALERT_2_C D-H Bond Without Acceptor N2   --H2N   .   Please Check

---

⚪ **Alert level G**

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   4 Note
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 .... 0.00019 Ang.
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   2 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records   2 Report
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   5 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .   Please Do !

---

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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 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
   4 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 22/08/2024; check.def file version of 21/08/2024

NOMOVE FORCED

Prob = 50
Temp = 150

-32 Y

PLATON-Oct 16 15:31:58 2024 - (220824)

Z 57   faces-xstr1656_flP b c a   R = 0.03   RES= 0   42 X