checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB3

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: MAB3

Bond precision: C-C = 0.0012 A   Wavelength=0.71075

Cell: a=9.0501(2)   b=9.1652(2)   c=9.5476(2)
               alpha=104.254(2)   beta=94.968(2)   gamma=103.538(2)
Temperature: 100 K

	Calculated	Reported
Volume	737.43(3)	737.43(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H20 N4, 2(B5 H4 O10)	C16 H20 N4, 2(B5 H4 O10)
Sum formula	C16 H28 B10 N4 O20	C16 H28 B10 N4 O20
Mr	704.52	704.52
Dx,g cm-3	1.587	1.586
Z	1	1
Mu (mm-1)	0.135	0.135
F000	362.0	362.0
F000'	362.24	
h,k,lmax	12,13,13	12,13,13
Nref	4493	4490
Tmin,Tmax	0.984,0.992	0.815,1.000
Tmin'	0.983	

Correction method= # Reported T Limits: Tmin=0.815 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999   Theta(max)= 30.507

R(reflections)= 0.0312(4220)   wR2(reflections)=
                                                 0.0890(4490)

S = 1.061   Npar= 243

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
```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....     2.10 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        3 Report
            1 -1  1,   0  2  1,   1 -2  2,
```

Alert level G
```
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)     0.002 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  O10      ..C3       .      2.90 Ang.
                                    1+x,y,z  =      1_655 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O10      ..C2       .      3.01 Ang.
                                    1+x,y,z  =      1_655 Check
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....       2 Note
            0  2  1,   1 -2  2,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     6.17 Note
            Predicted wR2: Based on SigI**2  1.44 or SHELX Weight  8.63
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       5 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by       3 Check
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   2 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
   4 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 06/01/2024; check.def file version of 05/01/2024

Datablock MAB3 - ellipsoid plot