checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

```
Bond precision:  C-C = 0.0052 A          Wavelength=0.71073

Cell:           a=10.1996(4)    b=19.6440(11)       c=12.5325(6)
                alpha=90        beta=113.734(3)     gamma=90
Temperature:    293 K

                Calculated                Reported
Volume          2298.7(2)                 2298.65(19)
Space group     P 21/n                    P21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula  C24 H28 N2 O8             C24 H28 N2 O8
Sum formula     C24 H28 N2 O8             C24 H28 N2 O8
Mr              472.48                    472.48
Dx,g cm-3       1.365                     1.365
Z               4                         4
Mu (mm-1)       0.103                     0.103
F000            1000.0                    1000.0
F000'           1000.56
h,k,lmax        12,23,15                  12,23,15
Nref            4206                      4170
Tmin,Tmax       0.988,0.990               0.965,0.990
Tmin'           0.965

Correction method= # Reported T Limits: Tmin=0.965 Tmax=0.990
AbsCorr = MULTI-SCAN

Data completeness= 0.991          Theta(max)= 25.370

R(reflections)= 0.0573( 2445)     wR2(reflections)= 0.1572( 4170)

S = 1.038                 Npar= 313
```

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

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 11 Note

Alert level C

PLAT199_ALERT_1_C Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_C Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00515 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X H2 ..H21 1.99 Ang.
x,y,z = 1_555 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.548 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 15 Report

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT793_ALERT_4_G Model has Chirality at C2 (Centro SPGR) R Verify
PLAT793_ALERT_4_G Model has Chirality at C5 (Centro SPGR) S Verify
PLAT793_ALERT_4_G Model has Chirality at C7 (Centro SPGR) R Verify
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 2 Info
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL/ 2018 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 11 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 Info

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

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

checkCIF publication errors

Alert level A

PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or
empty.

1 **ALERT level A** = Data missing that is essential or data in wrong format
1 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 18/09/2020; check.def file version of 20/08/2020

Datablock I - ellipsoid plot