checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 996

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: 996

```
Bond precision:   C-C = 0.0034 A          Wavelength=1.54184

Cell:             a=7.3438(1)     b=25.6051(3)         c=17.3123(3)
                  alpha=90        beta=100.256(1)      gamma=90
Temperature:      150 K

                 Calculated                 Reported
Volume           3203.37(8)                 3203.37(8)
Space group      P 21                       P 21
Hall group       P 2yb                      P 2yb
Moiety formula   C39 H52 N2 O2              C39 H52 N2 O2
Sum formula      C39 H52 N2 O2              C39 H52 N2 O2
Mr               580.83                     580.83
Dx,g cm-3        1.204                      1.204
Z                4                          4
Mu (mm-1)        0.561                      0.561
F000             1264.0                     1264.0
F000'            1267.28
h,k,lmax         9,32,21                    9,30,21
Nref             13478[ 6896]               10724
Tmin,Tmax        0.960,0.972                0.550,1.000
Tmin'            0.845

Correction method= # Reported T Limits: Tmin=0.550 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.56/0.80        Theta(max)= 76.600

R(reflections)= 0.0346( 10227)                wR2(reflections)=
                                              0.0904( 10724)
S = 1.035                 Npar= 790
```

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

```
PLAT414_ALERT_2_B Short Intra D-H..H-X       H28      ..H29      .       1.88 Ang.
                                                      x,y,z  =      1_555 Check
```

Author Response: The rule of van der Waals radii sum is fair for intermolecular interactions. Detected short distance H26...H29 is intramolecular. Its value also depends on other interactions except van der Waals forces.

Alert level C

```
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H19A     ..H33A     .       1.83 Ang.
                                                      x,y,z  =      1_555 Check
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H57A     ..H75A     .       1.89 Ang.
                                                      x,y,z  =      1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H50      ..H72      .       1.96 Ang.
                                                      x,y,z  =      1_555 Check
```

Author Response: The rule of van der Waals radii sum is fair for intermolecular interactions. Detected short distance H26...H29 is intramolecular. Its value also depends on other interactions except van der Waals forces.

```
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         11 Report
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage         67 %
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Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         22 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
              C39 H52 N2 O2
PLAT791_ALERT_4_G Model has Chirality at C5A         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C5B         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C8A         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C8B         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C9A         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C9B         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C10A        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C10B        (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C14A        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C14B        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C17A        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C17B        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C18A        (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C18B        (Sohnke SpGr)          S Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        537 Note
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PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         15 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.8 Low
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ           2 Units
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         17 Info
```

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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
  17 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 19/02/2022; check.def file version of 19/02/2022

Datablock 996 - ellipsoid plot