checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Form2_23mbb_sadnah16_ns16_bilpyether

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: Form2_23mbb_sadnah16_ns16_bilpyether

```
Bond precision:   C-C = 0.0100 A              Wavelength=0.71073

Cell:          a=11.8077(10)      b=15.0220(12)      c=19.3471(17)
               alpha=98.973(3)    beta=104.421(3)    gamma=111.029(3)
Temperature:   173 K

                 Calculated                   Reported
Volume           2985.8(4)                    2985.8(4)
Space group      P -1                         P -1
Hall group       -P 1                         -P 1
Moiety formula   C33 H36 N4 O6 [+ solvent]    1(C33 H36 N4 O6), 0.25[]
Sum formula      C33 H36 N4 O6 [+ solvent]    C33 H36 N4 O6
Mr               584.66                       584.66
Dx,g cm-3        1.301                        1.301
Z                4                            4
Mu (mm-1)        0.090                        0.090
F000             1240.0                       1240.0
F000'            1240.57
h,k,lmax         14,17,22                     14,17,22
Nref             10509                        10506
Tmin,Tmax        0.987,0.995                  0.617,0.746
Tmin'            0.987

Correction method= # Reported T Limits: Tmin=0.617 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000            Theta(max)= 24.998

                                                    wR2(reflections)=
R(reflections)= 0.0948( 4945)                       0.2974( 10506)

S = 1.029                      Npar= 808
```

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**

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
            Rint given   0.220

> **Author Response: The crystals are small and don't diffract well. Of several data collection attempts, this was the best data set we got.**

PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 ....   0.220 Report

> **Author Response: The crystals are small and don't diffract well. Of several data collection attempts, this was the data set we got.**

PLAT416_ALERT_2_B Short Intra D-H..H-D   H5   ..H6   .   1.85 Ang.
                                                     x,y,z =   1_555 Check

> **Author Response: Within the bilirubin molecule, there is three-center hydrogen bonding involving the amine (N-H) functional groups from two pyrroles and a carboxylic oxygen. The two amine functional groups are positioned closely together, creating the close contact.**

PLAT416_ALERT_2_B Short Intra D-H..H-D   H7   ..H8   .   1.84 Ang.
                                                     x,y,z =   1_555 Check

> **Author Response: Within the bilirubin molecule, there is three-center hydrogen bonding involving the amine (N-H) functional groups from two pyrroles and a carboxylic oxygen. The two amine functional groups are positioned closely together, creating the close contact.**

PLAT416_ALERT_2_B Short Intra D-H..H-D   H1   ..H2   .   1.84 Ang.
                                                     x,y,z =   1_555 Check

> **Author Response: Within the bilirubin molecule, there is three-center hydrogen bonding involving the amine (N-H) functional groups from two pyrroles and a carboxylic oxygen. The two amine functional groups are positioned closely together, creating the close contact.**

PLAT416_ALERT_2_B Short Intra D-H..H-D   H3A   ..H4   .   1.86 Ang.
                                                     x,y,z =   1_555 Check

Author Response: Within the bilirubin molecule, there is three-center hydrogen bonding involving the amine (N-H) functional groups from two pyrroles and a carboxylic oxygen. The two amine functional groups are positioned closely together, creating the close contact.

🟡 Alert level C

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PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..      47% Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................     0.30 Report
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N1        --C5       .     7.0 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C26       --C27      .     6.1 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C21       --C26      .    0.17 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C40 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for ..........      C40 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.00995 Ang.
PLAT368_ALERT_2_C Short  C(sp2)-C(sp2) Bond  C31       - C32      .    1.15 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H31       ..H32B     .    1.99 Ang.
                                            x,y,z  =      1_555 Check
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H46C      ..H46C     .    2.13 Ang.
                                         2-x,1-y,1-z  =      2_766 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...  -13.489 Report
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...   -0.328 Report
PLAT977_ALERT_2_C Check Negative Difference Density on H48B       .    -0.42 eA-3
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⚪ Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        8 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       20 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............       12 Report
              H5     H6     H7     H8     H9     H12    H1     H2     H3     H3A    H4
              H6A
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
              Calc: C33 H36 N4 O6
              Rep.: 1(C33 H36 N4 O6), 0.25[]
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large     0.12 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)     0.003 Degree
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records        1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records        5 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records        5 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used   0.0050 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)       5% Note
PLAT410_ALERT_2_G Short Intra H...H Contact  H59       ..H66C     .    2.09 Ang.
                                            x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O5        ..C57      .    2.97 Ang.
                                            x,y,z  =      1_555 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure      123 A**3
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      213 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed        ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).        2 Note
             0  1  0,   0  0  1,
PLAT930_ALERT_2_G FCF-based   Twin Law       [-1 3-5] Est.d BASF      0.78 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        1 Note
             0  1  0,
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..     50.0 Degree
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PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       3.42 Note
              Predicted wR2: Based on SigI**2  8.69 or SHELX Weight 30.09
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by         3 Check
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   0 ALERT level A = Most likely a serious problem – resolve or explain
   6 ALERT level B = A potentially serious problem, consider carefully
  14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  23 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  19 ALERT type 2 Indicator that the structure model may be wrong or deficient
  11 ALERT type 3 Indicator that the structure quality may be low
   7 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check
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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