checkCIF/PLATON report

Structure factors have been supplied for datablock(s) f-5026

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: f-5026

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Bond precision:    C-C = 0.0040 A             Wavelength=0.79990

Cell:              a=8.8500(18)        b=14.500(3)          c=23.750(5)
                   alpha=90            beta=99.66(3)        gamma=90
Temperature:       100 K

                   Calculated                 Reported
Volume             3004.5(11)                 3004.5(11)
Space group        P 21                       P 21
Hall group         P 2yb                      P 2yb
Moiety formula     C38 H34, C H2 Cl2          ?
Sum formula        C39 H36 Cl2                C78 H72 Cl4
Mr                 575.58                     1151.15
Dx,g cm-3          1.273                      1.272
Z                  4                          2
Mu (mm-1)          0.330                      0.336
F000               1216.0                     1216.0
F000'              1217.97
h,k,lmax           13,21,35                   13,20,31
Nref               20947[ 10838]              17697
Tmin,Tmax          0.968,0.977
Tmin'              0.967

Correction method= Not given

Data completeness= 1.63/0.84        Theta(max)= 36.653

                                               wR2(reflections)=
R(reflections)= 0.0420( 17174)                 0.1221( 17697)

S = 1.085                       Npar= 751
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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.

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🟠 **Alert level B**
PLAT035_ALERT_1_B _chemical_absolute_configuration Info Not Given   Please Do !
PLAT230_ALERT_2_B Hirshfeld Test Diff for   C31A   --C32A   .   7.2 s.u.

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🟡 **Alert level C**
STRVA01_ALERT_4_C   Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack   0.496
          From the CIF: _refine_ls_abs_structure_Flack_su   0.007
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .   0.961 Why?

> **Author Response: This is caused by the limited data collection strategy with
> the synchrotron facility.**

PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given   Please Do !
PLAT230_ALERT_2_C Hirshfeld Test Diff for   C32A   --C33A   .   5.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for   C34B   --C35B   .   5.8 s.u.
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.00403 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   221 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .   1 Check

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⚪ **Alert level G**
ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
                not performed for this radiation type.
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .   0.496 Note
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   2.00 Check
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.79990 Ang.
PLAT111_ALERT_2_G ADDSYM Detects New (Pseudo) Centre of Symmetry .   100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem   c   100 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space Group   P21/c Check
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =   3 Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   4 Note
PLAT791_ALERT_4_G Model has Chirality at C1A   (Sohnke SpGr)   S Verify
PLAT791_ALERT_4_G Model has Chirality at C1B   (Sohnke SpGr)   R Verify
PLAT791_ALERT_4_G Model has Chirality at C10A   (Sohnke SpGr)   R Verify
PLAT791_ALERT_4_G Model has Chirality at C12B   (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   1076 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....   1 Note
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ   4 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ   4 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   20 Info
PLAT984_ALERT_1_G The C-f'=   0.0033 Deviates from the B&C-Value 0.0043 Check
PLAT984_ALERT_1_G The Cl-f'=   0.1615 Deviates from the B&C-Value 0.1777 Check
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by   4 Check

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   0 **ALERT level A** = Most likely a serious problem – resolve or explain

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  2 ALERT level B = A potentially serious problem, consider carefully
  8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 22 ALERT level G = General information/check it is not something unexpected

  8 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
  5 ALERT type 3 Indicator that the structure quality may be low
 10 ALERT type 4 Improvement, methodology, query or suggestion
  2 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 13/07/2021; check.def file version of 13/07/2021

NOMOVE FORCED

Prob = 50
Temp = 100

52 Y

PLATON-Sep 17 09:57:33 2021 - (1307721)

Z 6   f-5026   P 21   R = 0.04   RES= 0   65 X