checkCIF/PLATON report

Structure factors have been supplied for datablock(s) zyfx1_a_pl

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: zyfx1_a_pl

Bond precision: C-C = 0.0042 A   Wavelength=1.34139

Cell: a=20.3486(7)   b=20.3486(7)   c=7.9296(2)
                  alpha=90   beta=90   gamma=90
Temperature: 150 K

                  Calculated   Reported
Volume   3283.4(2)   3283.4(2)
Space group   P -4 21 c   P -4 21 c
Hall group   P -4 2n   P -4 2n
Moiety formula   C22 H17 N O2 [+ solvent]   C22 H17 N O2
Sum formula   C22 H17 N O2 [+ solvent]   C22 H17 N O2
Mr   327.37   327.36
Dx,g cm-3   1.324   1.324
Z   8   8
Mu (mm-1)   0.430   0.430
F000   1376.0   1376.0
F000'   1379.03
h,k,lmax   25,25,9   25,25,9
Nref   3367[1907]   3356
Tmin,Tmax   0.805,0.950   0.747,1.000
Tmin'   0.796

Correction method= # Reported T Limits: Tmin=0.747 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.76/1.00   Theta(max)= 57.081

R(reflections)= 0.0654(3163)   wR2(reflections)=
                                                   0.1585(3356)

S = 1.114   Npar= 228

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

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
            a literature citation. This should be contained in the
            _exptl_absorpt_process_details field.
            Absorption correction given as multi-scan
STRVA01_ALERT_4_C   Flack parameter is too small
            From the CIF: _refine_ls_abs_structure_Flack   -0.500
            From the CIF: _refine_ls_abs_structure_Flack_su   0.500
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.00421 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   5 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .   1 Check

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   1 Report
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .   0.500 Report
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure   25 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   42 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed   ! Info
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   1 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .   0.20 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File   5 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   0 Info

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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 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
   6 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 06/07/2023; check.def file version of 30/06/2023