checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_ydg_lcf_oh_002_0m_a

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: mo_ydg_lcf_oh_002_0m_a

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Bond precision:   C-C = 0.0070 A           Wavelength=0.71073

Cell:           a=5.3349(10)       b=9.7052(18)      c=9.9046(18)
                alpha=65.757(6)    beta=79.472(6)    gamma=75.882(6)
Temperature:    303 K

                Calculated                 Reported
Volume          451.49(15)                 451.49(15)
Space group     P 1                        P 1
Hall group      P 1                        P 1
Moiety formula  C17 H20 F N6 O4            C17 H20 F N6 O4
Sum formula     C17 H20 F N6 O4            C17 H20 F N6 O4
Mr              391.39                     391.39
Dx,g cm-3       1.439                      1.439
Z               1                          1
Mu (mm-1)       0.112                      0.112
F000            205.0                      205.0
F000'           205.10
h,k,lmax        6,12,12                    6,12,12
Nref            4178[ 2089]                3949
Tmin,Tmax       0.981,0.991                0.594,0.746
Tmin'           0.954

Correction method= # Reported T Limits: Tmin=0.594 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.89/0.95        Theta(max)= 27.597

R(reflections)= 0.0490( 2764)                wR2(reflections)=
                                             0.1307( 3949)
S = 1.028                  Npar= 257
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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.

Alert level C

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STRVA01_ALERT_4_C           Flack test results are meaningless.
          From the CIF: _refine_ls_abs_structure_Flack   -0.200
          From the CIF: _refine_ls_abs_structure_Flack_su    0.600
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............      0.007 Ang.
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N4       --H4A      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N19      --H19A     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N19      --H19B     .     Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          3 Report
               6  4  0,   5  7  0,   5  7  2,
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Alert level G

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PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          8 Report
             H2    H4    H4A   H5    H6A   H6B   H19A  H19B
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .      0.600 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.006 Degree
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O1       .      109.8 Degree
PLAT791_ALERT_4_G Model has Chirality at C2         (Sohncke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C3         (Sohncke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C10        (Sohncke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C11        (Sohncke SpGr)          R Verify
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
               0  0  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         13 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .       0.50 Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      1.796 Note
             Predicted wR2: Based on SigI**2  7.28 or SHELX Weight 12.72
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
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
14 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
7 ALERT type 4 Improvement, methodology, query or suggestion
3 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 13/05/2024; check.def file version of 04/05/2024

Datablock mo_ydg_lcf_oh_002_0m_a - ellipsoid plot