checkCIF/PLATON report

Structure factors have been supplied for datablock(s) new-jg571_twin1

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: new-jg571_twin1

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Bond precision:   C-C = 0.0055 A            Wavelength=0.71073

Cell:          a=6.6189(2)        b=10.0399(4)      c=18.8507(7)
               alpha=83.114(3)   beta=80.511(3)   gamma=81.261(3)
Temperature:   293 K

                 Calculated                    Reported
Volume         1215.41(8)                     1215.40(8)
Space group    P -1                           P -1
Hall group     -P 1                           -P 1
Moiety formula C31 H29 N5 O                   C31 H29 N5 O
Sum formula    C31 H29 N5 O                   C31 H29 N5 O
Mr             487.59                         487.59
Dx,g cm-3      1.332                          1.332
Z              2                              2
Mu (mm-1)      0.083                          0.083
F000           516.0                          516.0
F000'          516.18
h,k,lmax       7,12,22                        7,12,22
Nref           4388                           6194
Tmin,Tmax      0.980,0.996                    0.875,1.000
Tmin'          0.975

Correction method= # Reported T Limits: Tmin=0.875 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.412           Theta(max)= 25.242

R(reflections)= 0.0617( 5834)      wR2(reflections)= 0.1497( 6194)

S = 1.194                 Npar= 335
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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 C

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PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00552 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......    2.964 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         2 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .         2 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .    10.23 Check
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Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         1 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)    0.003 Degree
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)       293 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C30       ..C30         3.09 Ang.
                                              1-x,1-y,1-z  =     2_666 Check
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..         ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still     90% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         1 Note
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 0 0 1)       Est.d BASF     0.32 Check
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         4 Note
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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
  10 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   7 ALERT type 3 Indicator that the structure quality may be low
   1 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 22/12/2019; check.def file version of 13/12/2019