checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ye393P-1_as

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: ye393P-1_as

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Bond precision:   C-C = 0.0080 A          Wavelength=0.71073

Cell:               a=11.5152(6)      b=8.3196(4)      c=44.227(2)
                    alpha=90          beta=90          gamma=90
Temperature:        296 K

                 Calculated                Reported
Volume           4237.0(4)                 4237.0(4)
Space group      P b c a                   P b c a
Hall group       -P 2ac 2ab                -P 2ac 2ab
Moiety formula   C25 H24 O4                C25 H24 O4
Sum formula      C25 H24 O4                C25 H24 O4
Mr               388.44                    388.44
Dx,g cm-3        1.218                     1.218
Z                8                         8
Mu (mm-1)        0.082                     0.082
F000             1648.0                    1648.0
F000'            1648.81
h,k,lmax         13,9,51                   13,9,51
Nref             3434                      3432
Tmin,Tmax        0.988,0.991               0.789,1.000
Tmin'            0.988

Correction method= # Reported T Limits: Tmin=0.789 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999           Theta(max)= 24.248

R(reflections)= 0.1075( 2065)                wR2(reflections)=
                                             0.2736( 3432)
S = 1.087                Npar= 313
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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 B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.184
PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 ..... 0.184 Report

Alert level C

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5778
PLAT082_ALERT_2_C High R1 Value ..... 0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.27 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference O27 --C26 . 0.17 Ang.
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00804 Ang.
PLAT368_ALERT_2_C Short C(sp2)-C(sp2) Bond C24 - C25 . 1.22 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 39.938 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 5.962 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.581 Check

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 15 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 10 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 8.13 Why ?
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 17% Note
PLAT793_ALERT_4_G Model has Chirality at C12 (Centro SPGR) S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 213 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by . 1 Units
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 48.5 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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
5 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 12/09/2022; check.def file version of 09/08/2022

Datablock ye393P-1_as - ellipsoid plot