checkCIF/PLATON report

Structure factors have been supplied for datablock(s) lsf_03_benz_ts

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: lsf_03_benz_ts

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Bond precision:   C-C = 0.0068 A          Wavelength=0.71073

Cell:             a=10.1989(5)     b=8.7455(4)         c=15.8721(9)
                  alpha=90         beta=99.068(5)      gamma=90
Temperature:      298 K

                 Calculated                Reported
Volume           1398.01(12)               1398.01(12)
Space group      P 21                      P 21
Hall group       P 2yb                     P 2yb
Moiety formula   C26 H31 N O12             ?
Sum formula      C26 H31 N O12             C26 H31 N O12
Mr               549.52                    549.52
Dx,g cm-3        1.305                     1.305
Z                2                         2
Mu (mm-1)        0.104                     0.104
F000             580.0                     580.0
F000'            580.37
h,k,lmax         14,12,21                  13,11,21
Nref             7606[ 4039]               15990
Tmin,Tmax        0.963,0.990               0.784,1.000
Tmin'            0.959

Correction method= # Reported T Limits: Tmin=0.784 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 3.96/2.10        Theta(max)= 29.275

R(reflections)= 0.0458( 8178)                wR2(reflections)=
                                             0.1185( 15990)
S = 0.795                 Npar= 368
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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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GOODF01_ALERT_2_C  The least squares goodness of fit parameter lies
           outside the range 0.80 <> 2.00
           Goodness of fit given =      0.795
STRVA01_ALERT_4_C          Flack test results are meaningless.
          From the CIF: _refine_ls_abs_structure_Flack   -0.100
          From the CIF: _refine_ls_abs_structure_Flack_su    0.600
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.2 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range        4.6 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        4.3 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C21 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C19 Check
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C19      --C24      .       1.36 Ang.
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00675 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H18B     ..O8       .       2.62 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.227 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          9 Note
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Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .      0.600 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O1A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1B        Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         3% Note
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O10            108.7 Degree
PLAT791_ALERT_4_G Model has Chirality at C6          (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C7          (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C10         (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C13         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C14         (Sohnke SpGr)          S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        292 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects 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        262 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .       0.60 Check
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.3 Low
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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
  14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  18 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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 10 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
 13 ALERT type 4 Improvement, methodology, query or suggestion
  1 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

Datablock lsf_03_benz_ts - ellipsoid plot