checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ca301020_1_1

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: ca301020_1_1

Bond precision: C-C = 0.0046 A   Wavelength=1.54184

Cell: a=12.8695(1)   b=11.9813(1)   c=17.9543(2)
                alpha=90   beta=98.143(1)   gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2740.52(4)	2740.52(4)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C28 H37 Br N2 O Si	C28 H37 Br N2 O Si
Sum formula	C28 H37 Br N2 O Si	C28 H37 Br N2 O Si
Mr	525.59	525.59
Dx,g cm-3	1.274	1.274
Z	4	4
Mu (mm-1)	2.622	2.622
F000	1104.0	1104.0
F000'	1104.63	
h,k,lmax	16,15,22	16,15,22
Nref	6005	5963
Tmin,Tmax	0.450,0.896	0.313,1.000
Tmin'	0.408	

Correction method= # Reported T Limits: Tmin=0.313 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.993   Theta(max)= 80.082

R(reflections)= 0.0526(5594)   wR2(reflections)= 0.1449(5963)

S = 1.048   Npar= 328

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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PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....        3.09 Report
PLAT213_ALERT_2_C Atom C24A            has ADP max/min Ratio .....          3.5 oblate
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range          3.2 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1   H   Uiso(max)/Uiso(min) Range         4.2 Ratio
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......        2.717 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.21A    From C4               2.22 eA-3
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite           7 Note
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large         5.71 Why ?
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing ..............     0.00010 Ang.
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records           1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records           3 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records           1 Report
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )            9% Note
PLAT721_ALERT_1_G Bond    Calc       0.97000, Rep      0.96000 Dev...     0.01 Ang.
          C25A      -H25D              1.555   1.555 ........    #   80 Check
PLAT793_ALERT_4_G Model has Chirality at C10          (Centro SPGR)           R Verify
PLAT793_ALERT_4_G Model has Chirality at C11          (Centro SPGR)           S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         38 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         42 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          2 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
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   7 ALERT type 4 Improvement, methodology, query or suggestion
   0 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 18/09/2020; check.def file version of 20/08/2020