checkCIF/PLATON report

Structure factors have been supplied for datablock(s) is98

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: is98

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Bond precision:   C-C = 0.0120 A          Wavelength=0.71073

Cell:             a=21.3396(16)     b=13.0859(11)      c=15.3330(12)
                  alpha=90          beta=90.493(3)     gamma=90
Temperature:      150 K
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	Calculated	Reported
Volume	4281.6(6)	4281.5(6)
Space group	P c	P 1 c 1
Hall group	P -2yc	P -2yc
Moiety formula	I9 Sb2, 3(C7 H9 Br N)	I9 Sb2, 3(C7 H9 Br N)
Sum formula	C21 H27 Br3 I9 N3 Sb2	C21 H27 Br3 I9 N3 Sb2
Mr	1946.78	1946.78
Dx,g cm-3	3.020	3.020
Z	4	4
Mu (mm-1)	10.569	10.569
F000	3432.0	3432.0
F000'	3408.58	
h,k,lmax	29,18,21	29,18,21
Nref	24128[12073]	24057
Tmin,Tmax	0.275,0.728	0.509,0.746
Tmin'	0.254	

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Correction method= # Reported T Limits: Tmin=0.509 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.99/1.00        Theta(max)= 29.619

R(reflections)= 0.0259( 22870)                wR2(reflections)=
                                              0.0496( 24057)
S = 1.121                  Npar= 691
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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

```
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............      0.012 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          9 Report
                0  2  0,   6  0  0,  -3  3  1,   3  3  1,   0  0  2,   3  3  3,
               -4  0  4,  -2  0  4,   2  0  4,
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          1 Check
                0  1-13,
PLAT977_ALERT_2_C Check Negative Difference Density on H18       .      -0.34 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H25       .      -0.34 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H27A      .      -0.34 eA-3
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Alert level G

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PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       9.39 Why ?
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem        21        100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem         b        100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem         C         88 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New  Space Group      Pca21 Check
            Check Model Parameter Symmetry for Reflection Data Support
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  I4       --Sb1      .        8.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  I4       --Sb2      .       11.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  I5       --Sb1      .       12.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  I5       --Sb2      .       12.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  I6       --Sb1      .       15.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  I6       --Sb2      .       13.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  I13      --Sb3      .       11.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  I13      --Sb4      .       12.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  I14      --Sb3      .       10.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  I14      --Sb4      .        8.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  I15      --Sb3      .       13.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  I15      --Sb4      .       17.0 s.u.
PLAT434_ALERT_2_G Short Inter HL..HL Contact I5       ..Br2      .       3.59 Ang.
                                                      x,y,z  =      1_555 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact I13      ..Br5      .       3.58 Ang.
                                                      x,y,z  =      1_555 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Sb1       (III)     .       3.12 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Sb2       (III)     .       3.09 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Sb3       (III)     .       3.09 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Sb4       (III)     .       3.12 Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
                1  0  0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         15 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
                6  0  0,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       1.51 Note
            Predicted wR2: Based on SigI**2  3.30 or SHELX Weight  4.50
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

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  6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 28 ALERT level G = General information/check it is not something unexpected

  0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 23 ALERT type 2 Indicator that the structure model may be wrong or deficient
  5 ALERT type 3 Indicator that the structure quality may be low
  1 ALERT type 4 Improvement, methodology, query or suggestion
  5 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 06/01/2024; check.def file version of 05/01/2024

Datablock is98 - ellipsoid plot