checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1057_0m_a

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: 1057_0m_a

```
Bond precision:  C-C = 0.0290 A          Wavelength=0.71073

Cell:            a=12.556(18)    b=16.427(17)       c=16.664(17)
                 alpha=90        beta=109.46(5)     gamma=90
Temperature:     293 K
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	Calculated	Reported
Volume	3241(7)	3241(7)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C25 H18 Br5 F4 O7 Sb	?
Sum formula	C25 H18 Br5 F4 O7 Sb	C25 H18 Br5 F4 O7 Sb
Mr	1027.65	1027.69
Dx,g cm-3	2.106	2.106
Z	4	4
Mu (mm-1)	7.078	7.079
F000	1944.0	1944.0
F000’	1937.30	
h,k,lmax	11,15,15	11,15,15
Nref	2739	2664
Tmin,Tmax	0.050,0.159	0.097,0.261
Tmin’	0.010	

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Correction method= # Reported T Limits: Tmin=0.097 Tmax=0.261
AbsCorr = MULTI-SCAN

Data completeness= 0.973          Theta(max)= 19.323

R(reflections)= 0.0601( 2158)     wR2(reflections)= 0.1692( 2664)

S = 1.079                 Npar= 383
```

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 A

```
THETM01_ALERT_3_A  The value of sine(theta_max)/wavelength is less than 0.550
           Calculated sin(theta_max)/wavelength =    0.4656
PLAT234_ALERT_4_A Large Hirshfeld Difference C4       --C5       .       0.32 Ang.
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Alert level B

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PLAT088_ALERT_3_B Poor Data / Parameter Ratio ...................       6.96 Note
PLAT342_ALERT_3_B Low Bond Precision on  C-C Bonds ..............      0.029 Ang.
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).         11 Note
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Alert level C

```
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.972 Why?
PLAT031_ALERT_4_C Refined Extinction Parameter Within Range ......      3.000 Sigma
PLAT148_ALERT_3_C s.u. on the      a    - Axis is (Too) Large ....      0.018 Ang.
PLAT148_ALERT_3_C s.u. on the      b    - Axis is (Too) Large ....     0.0170 Ang.
PLAT148_ALERT_3_C s.u. on the      c    - Axis is (Too) Large ....      0.017 Ang.
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        3.5 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C18      --C19      .       0.20 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O6 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         O1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         O2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         O3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C5 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C8 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C9 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C15 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C18 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C19 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C25 Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C1       -C6             1.35 Ang.
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C11      -C16            1.37 Ang.
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C21      -C26            1.36 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact  F4       ..O7       .       2.86 Ang.
                                          1-x,1-y,1-z  =      3_666 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.466         67 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
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Alert level G

```
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          4 Report
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....       0.62 mm
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      39.91 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Br1      ..Br3             3.56 Ang.
                                       -1+x,3/2-y,-1/2+z  =      4_475 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Br4      ..Br5             3.45 Ang.
                                             1+x,y,z  =      1_655 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        24 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        65% Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          1 Note
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2 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
25 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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 12 ALERT level G = General information/check it is not something unexpected

  3 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
 11 ALERT type 3 Indicator that the structure quality may be low
  5 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 03/05/2019; check.def file version of 29/04/2019

Datablock 1057_0m_a - ellipsoid plot