# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) platon_sq

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: platon_sq

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Bond precision:  C-C = 0.0126 A          Wavelength=0.71073

Cell:          a=12.484(14)       b=13.650(15)     c=13.671(17)
               alpha=102.29(3)    beta=114.56(5)   gamma=96.38(3)
Temperature:   293 K
```

| | Calculated | Reported |
|---|---|---|
| Volume | 2017(4) | 2017(4) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C35 H20 Br3 F8 O7 Sb [+ solvent] | ? |
| Sum formula | C35 H20 Br3 F8 O7 Sb [+ solvent] | C35 H20 Br3 F8 O7 Sb [+ SOLVENT] |
| Mr | 1065.97 | 1065.99 |
| Dx,g cm-3 | 1.755 | 1.755 |
| Z | 2 | 2 |
| Mu (mm-1) | 3.736 | 3.735 |
| F000 | 1028.0 | 1028.0 |
| F000’ | 1025.78 | |
| h,k,lmax | 12,14,14 | 12,14,14 |
| Nref | 4631 | 4557 |
| Tmin,Tmax | 0.617,0.715 | 0.455,0.730 |
| Tmin’ | 0.389 | |

```
Correction method= # Reported T Limits: Tmin=0.455 Tmax=0.730
AbsCorr = MULTI-SCAN

Data completeness= 0.984          Theta(max)= 21.514

R(reflections)= 0.0386( 3896)     wR2(reflections)= 0.0993( 4557)

S = 1.031                 Npar= 501
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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.

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## Alert level A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5160

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## Alert level B

PLAT230_ALERT_2_B Hirshfeld Test Diff for F1 --C32 . 7.2 s.u.
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 19 Note

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## Alert level C

PLAT088_ALERT_3_C Poor Data / Parameter Ratio ..... 9.10 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 3.52 Report
PLAT148_ALERT_3_C s.u. on the a - Axis is (Too) Large .... 0.014 Ang.
PLAT148_ALERT_3_C s.u. on the b - Axis is (Too) Large .... 0.015 Ang.
PLAT148_ALERT_3_C s.u. on the c - Axis is (Too) Large .... 0.017 Ang.
PLAT213_ALERT_2_C Atom F2 has ADP max/min Ratio ..... 3.2 prolat
PLAT213_ALERT_2_C Atom F7 has ADP max/min Ratio ..... 3.2 prolat
PLAT213_ALERT_2_C Atom F8 has ADP max/min Ratio ..... 3.8 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference F5B --C46 . 0.25 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C32 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C33 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C34 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C35 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C41 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C43 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C44 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C45 Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C31 -C36 1.37 Ang.
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01256 Ang.
PLAT434_ALERT_2_C Short Inter HL..HL Contact F3 ..F5B 2.55 Ang.
x,y,-1+z = 1_554 Check
PLAT480_ALERT_4_C Long H...A H-Bond Reported H14 ..F2 . 2.62 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.516 55 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

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## Alert level G

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum C35 H20 Br3 F8 O7 Sb [+ solvent]
TEST: Compare cell contents of formula and atom_site data

| atom | Z*formula | cif sites | diff |
|---|---|---|---|
| C | 70.00 | 70.00 | 0.00 |
| H | 40.00 | 40.00 | 0.00 |
| Br | 6.00 | 6.00 | 0.00 |
| F | 16.00 | 16.00 | 0.00 |
| O | 14.00 | 14.00 | 0.00 |
| Sb | 2.00 | 2.00 | 0.00 |
| [+ | 2.00 | 0.00 | 2.00 |
| solve | 2.00 | 0.00 | 2.00 |

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.69 Why ?

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PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         2% Note
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        248 A**3
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed           ! Info
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         75% Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          7 Note
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  1 ALERT level A = Most likely a serious problem - resolve or explain
  2 ALERT level B = A potentially serious problem, consider carefully
 24 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 11 ALERT level G = General information/check it is not something unexpected

  5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 19 ALERT type 2 Indicator that the structure model may be wrong or deficient
 10 ALERT type 3 Indicator that the structure quality may be low
  4 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.

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**PLATON version of 03/05/2019; check.def file version of 29/04/2019**

**Datablock platon_sq** - ellipsoid plot