checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 111

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: 111

[(^{Ph,tBu}BCB)($SbCl_2$)](**1**)

Bond precision: C-C = 0.0082 A Wavelength=1.54184

Cell: a=11.2125(3) b=13.5169(2) c=21.8376(4)
alpha=90 beta=96.970(2) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	3285.21(12)	3285.21(12)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C26 H32 B Cl2 N4 Sb, C7 H8	C26 H32 B Cl2 N4 Sb, C7 H8
Sum formula	C33 H40 B Cl2 N4 Sb	C33 H40 B Cl2 N4 Sb
Mr	696.16	696.15
Dx,g cm-3	1.408	1.407
Z	4	4
Mu (mm-1)	8.366	8.366
F000	1424.0	1424.0
F000'	1429.73	
h,k,lmax	14,17,27	14,17,27
Nref	6851	6746
Tmin,Tmax	0.421,0.433	0.813,1.000
Tmin'	0.163	

Correction method= # Reported T Limits: Tmin=0.813 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.985 Theta(max)= 76.022

R(reflections)= 0.0408(5408) wR2(reflections)= 0.0950(6746)

S = 1.009 Npar= 377

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

```
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C29      --C30      .       0.20 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C11 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00819 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.090 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          3 Report
             -11  2 16, -11  0 17,  -9  1 19,
```

Alert level G

```
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        101 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         10 Note
             -12  2 16, -12  4 14, -12  3 15, -12  0 16, -13  3 12,  -9  1 19,
             -13  2 13, -10  3 21, -11  2 16, -11  0 17,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.5 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       1.50 Note
             Predicted wR2: Based on SigI**2  6.35 or SHELX Weight  9.69
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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

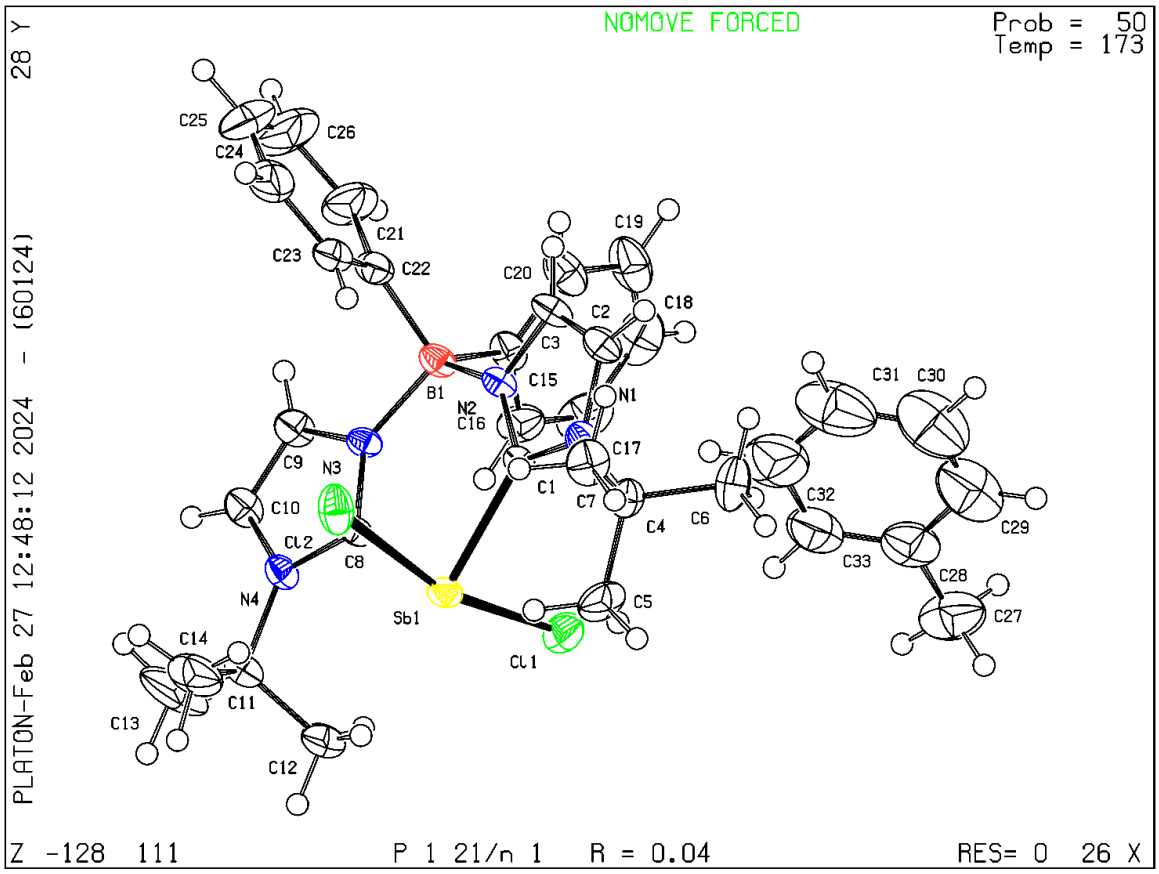
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 111 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 1 [(^{Ph,tBu}BCB)Sb](**2**):

```
Bond precision:   C-C = 0.0123 A          Wavelength=1.54184

Cell:             a=11.1261(3)     b=11.3079(2)       c=39.7146(9)
                  alpha=90         beta=97.649(2)     gamma=90
Temperature:      173 K
```

	Calculated	Reported
Volume	4952.2(2)	4952.1(2)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C26 H32 B N4 Sb	2(C26 H32 B N4 Sb)
Sum formula	C26 H32 B N4 Sb	C52 H64 B2 N8 Sb2
Mr	533.13	1066.23
Dx,g cm-3	1.430	1.430
Z	8	4
Mu (mm-1)	8.981	8.981
F000	2176.0	2176.0
F000'	2180.57	
h,k,lmax	14,14,49	13,14,49
Nref	10316	10451
Tmin,Tmax	0.028,0.914	0.746,1.000
Tmin'	0.004	

```
Correction method= # Reported T Limits: Tmin=0.746 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.013          Theta(max)= 76.010

R(reflections)= 0.0645( 8454)                wR2(reflections)=
                                             0.1916( 10451)
S = 1.083                 Npar= 590
```

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 ..... 0.01228 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 13 Report
PLAT920_ALERT_1_C Theta(Max) in CIF and FCF Differ by ..... 0.33 Degree

Alert level G

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 2 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 27.50 Why ?
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 120 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 !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 161 Note
PLAT931_ALERT_5_G CIFcalcFCF Twin Law [1 0 2] Est.d BASF 0.16 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 12 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.8 Low

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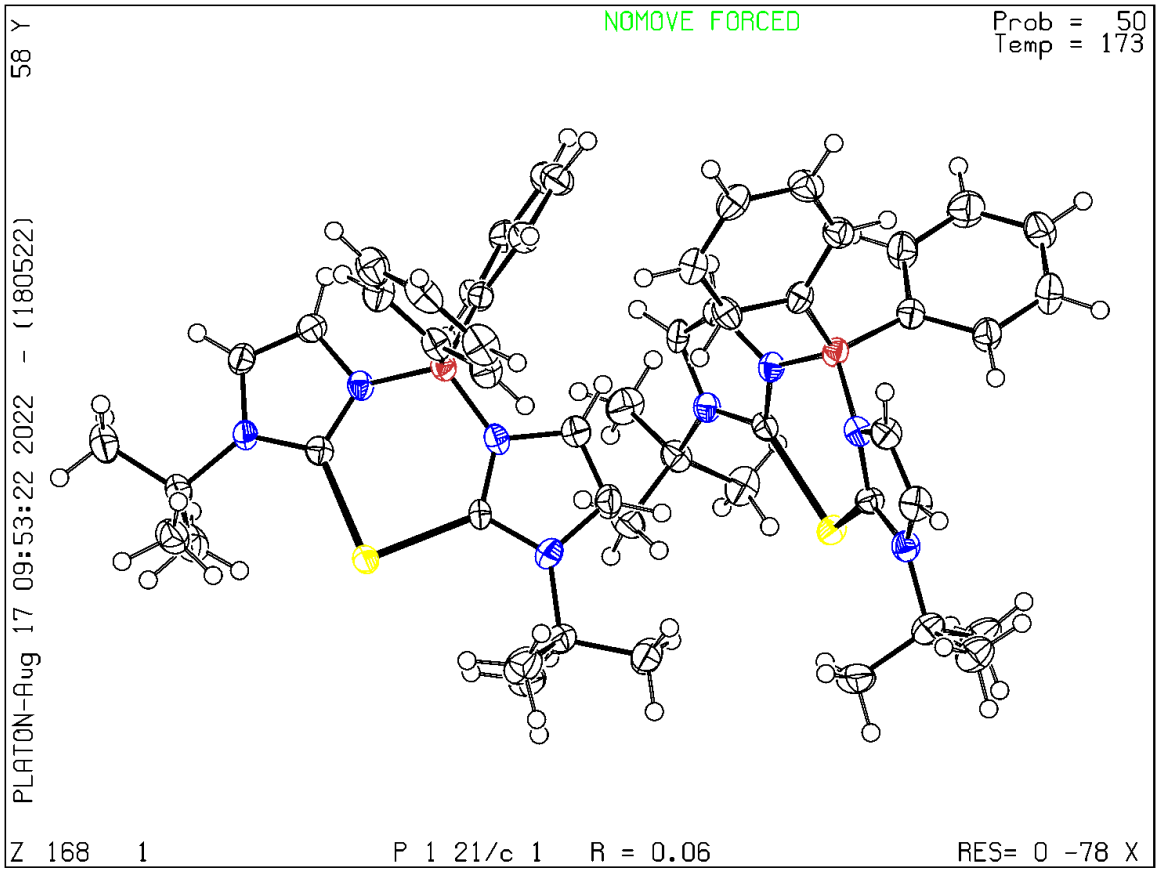
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 18/05/2022; check.def file version of 17/05/2022

Datablock 1 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) zjy_4_781_3_auto

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: zjy_4_781_3_auto

(^{Ph,tBu}BCB)Sb[Rh(CO)(acac)] (**3**)

Bond precision: C-C = 0.0512 A Wavelength=1.54184

Cell: a=15.4494(8) b=8.3395(5) c=30.0518(11)
alpha=90 beta=92.596(5) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	3867.9(3)	3867.9(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C32 H38 B N4 O3 Rh Sb	C32 H38 B N4 O3 Rh Sb
Sum formula	C32 H38 B N4 O3 Rh Sb	C32 H38 B N4 O3 Rh Sb
Mr	762.14	762.13
Dx,g cm-3	1.309	1.309
Z	4	4
Mu (mm-1)	9.240	9.240
F000	1532.0	1532.0
F000'	1535.88	
h,k,lmax	19,10,37	19,9,37
Nref	8187	6046
Tmin,Tmax	0.895,0.912	0.640,1.000
Tmin'	0.397	

Correction method= # Reported T Limits: Tmin=0.640 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.738 Theta(max)= 76.883

R(reflections)= 0.1772(4739) wR2(reflections)= 0.4990(6046)

S = 1.095 Npar= 387

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.

While the refinement quality is limited, the crystallographic data clearly confirm the atom connectivity and molecular geometry

---

Alert level A

```
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low .      0.789 Why?
PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ..................       0.50 Report
PLAT971_ALERT_2_A Check Calcd Resid. Dens.  1.48Ang From O2             7.81 eA-3
PLAT971_ALERT_2_A Check Calcd Resid. Dens.  1.89Ang From N1             5.57 eA-3
PLAT971_ALERT_2_A Check Calcd Resid. Dens.  2.52Ang From C5             5.32 eA-3
PLAT971_ALERT_2_A Check Calcd Resid. Dens.  2.72Ang From C8             3.91 eA-3
PLAT971_ALERT_2_A Check Calcd Resid. Dens.  1.43Ang From O2             3.70 eA-3
PLAT971_ALERT_2_A Check Calcd Resid. Dens.  1.23Ang From C4             3.58 eA-3
```

Alert level B

```
PLAT082_ALERT_2_B High R1 Value .................................       0.18 Report
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density      5.50 eA-3
PLAT342_ALERT_3_B Low Bond Precision on  C-C Bonds ..............    0.05125 Ang.
PLAT601_ALERT_2_B Unit-Cell Contains Solvent Accessible VOIDS .LE.       188 Ang**3
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L=    0.600      1468 Report
                  0  2  0,   0  4  0,   0  6  0,   1  1  0,   1  2  0,   1  3  0,
                  1  4  0,   1  5  0,   1  9  0,   2  3  0,   2  9  0,   3  1  0,
                  3  8  0,   3  9  0,   4  9  0,   5  9  0,   6  4  0,   6  9  0,
                 14  6  0,  16  5  0, -16  5  1, -14  6  1, -11  0  1, -11  6  1,
                 -7  9  1,  -6  9  1,  -5  9  1,  -4  8  1,  -4  9  1,  -3  8  1,
                     ( 1438 More Missing: see the .ckf listing file)
PLAT925_ALERT_1_B The Reported and Calculated Rho(max) Differ by .      2.31 eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens.  1.67Ang From C7             3.25 eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens.  1.71Ang From C3             3.06 eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens.  2.89Ang From O3             3.04 eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens.  1.32Ang From C9             2.55 eA-3
PLAT972_ALERT_2_B Check Calcd Resid. Dens.  1.73Ang From C21           -2.69 eA-3
```

Alert level C

```
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
          The relevant atom site should be identified.
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....      2.90 Report
PLAT234_ALERT_4_C Large Hirshfeld Difference Rh1      --O2       .      0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N2       --B1       .      0.20 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C10 Check
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H16A     ..H16A     .      2.13 Ang.
                                          1-x,1-y,1-z  =      3_666 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     16.528 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      5.728 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.394 Check
```

```
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          1 Check
                2  0  0,
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          1 Check
                3  2  2,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.11Ang From Rh1              2.21 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.51Ang From C10              2.07 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  2.00Ang From C8               2.05 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.18Ang From C13              1.94 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.54Ang From Sb1              1.89 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.27Ang From Sb1              1.85 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.26Ang From Rh1              1.77 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.32Ang From Rh1              1.74 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.74Ang From O2              -2.16 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.78Ang From C29             -1.95 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.93Ang From Sb1             -1.95 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.94Ang From C27             -1.95 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.95Ang From C5              -1.92 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.73Ang From C22             -1.86 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.79Ang From C12             -1.83 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  2.20Ang From C3              -1.68 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.46Ang From O2              -1.66 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.87Ang From C8              -1.61 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.73Ang From Sb1             -1.60 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.97Ang From C9              -1.60 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.64Ang From O3              -1.59 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  2.21Ang From C22             -1.58 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  2.40Ang From C17             -1.58 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.77Ang From Rh1             -1.55 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H1A       .       -0.34 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H1C       .       -0.47 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H5B       .       -0.51 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H5C       .       -0.64 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H11A      .       -0.31 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H11C      .       -0.56 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H15B      .       -0.40 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H16C      .       -0.55 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H22       .       -0.50 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H23       .       -0.93 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H29       .       -1.02 eA-3
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          7 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms         20 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.16 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     643.91 Why ?
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          4 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          4 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0010 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0010 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0010 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0010 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par     0.0020 Report
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PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar     0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par     0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0005 Report
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for         C3 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       287 Note
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min)[Deg]=      3.16 Note
                  0  0  2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       554 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         2 Note
                  1  0  1,  -1  0  3,
PLAT930_ALERT_2_G FCF-based   Twin Law ( 1 0-1)         Est.d BASF      0.47 Check
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 1 0-1)         Est.d BASF      0.47 Check
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       2.2 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     7.066 Note
              Predicted wR2: Based on SigI**2  7.06 or SHELX Weight 45.57
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
```

```
   8 ALERT level A = Most likely a serious problem - resolve or explain
  11 ALERT level B = A potentially serious problem, consider carefully
  46 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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  59 ALERT type 2 Indicator that the structure model may be wrong or deficient
  21 ALERT type 3 Indicator that the structure quality may be low
   9 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

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PLATON version of 26/09/2025; check.def file version of 20/09/2025

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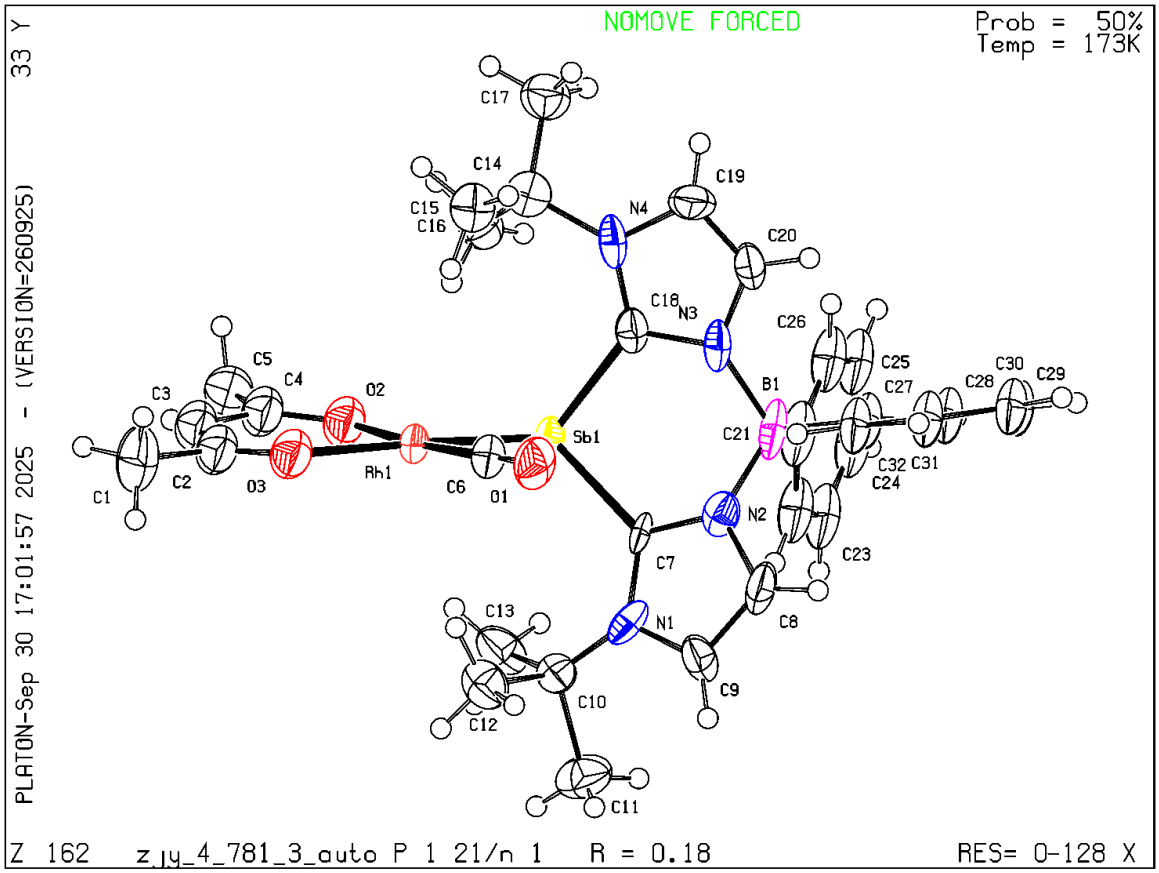
duplicate check

No duplication found

Datablock zjy_4_781_3_auto - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 222

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: 222

(^{Ph,tBu}BCB)Sb[PdCl(η^3-allyl)]$_2$ (**4**)

Bond precision: C-C = 0.0081 A Wavelength=1.54184

Cell: a=13.35437(5) b=13.35437(5) c=43.1985(3)
alpha=90 beta=90 gamma=90

Temperature: 173 K

	Calculated	Reported
Volume	7703.99(8)	7703.99(7)
Space group	P 43 21 2	P 43 21 2
Hall group	P 4nw 2abw	P 4nw 2abw
Moiety formula	C32 H42 B Cl2 N4 Pd2 Sb [+ solvent]	C32 H42 B Cl2 N4 Pd2 Sb
Sum formula	C32 H42 B Cl2 N4 Pd2 Sb [+ solvent]	C32 H42 B Cl2 N4 Pd2 Sb
Mr	898.97	898.95
Dx,g cm-3	1.550	1.550
Z	8	8
Mu (mm-1)	14.436	14.436
F000	3552.0	3552.0
F000'	3566.78	
h,k,lmax	16,16,54	16,16,54
Nref	8144[4718]	8038
Tmin,Tmax	0.295,0.236	0.574,1.000
Tmin'	0.189	

Correction method= # Reported T Limits: Tmin=0.574 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.70/0.99 Theta(max)= 76.931

R(reflections)= 0.0248(7896) wR2(reflections)= 0.0563(8038)

S = 1.061 Npar= 405

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

```
PLAT213_ALERT_2_C Atom C27            has ADP max/min Ratio .....       3.1 prolat
PLAT213_ALERT_2_C Atom C28            has ADP max/min Ratio .....       3.5 prolat
PLAT213_ALERT_2_C Atom C29            has ADP max/min Ratio .....       3.5 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range      4.7 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C29 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       Pd1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       Pd2 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.00805 Ang.
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        10 Note
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     11.71 Why ?
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............   0.00030 Ang.
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         6 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         1 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par    0.0001 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar    0.0002 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        5% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H19A     ..H27C     .      2.09 Ang.
                                                    x,y,z  =      1_555 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure       199 A**3
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        21 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed         ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        39 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         2 Note
               -6 15 14,   0  1  4,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     3.312 Note
             Predicted wR2: Based on SigI**2  1.69 or SHELX Weight  5.30
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
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
16 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

```
12 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
 6 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check
```

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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

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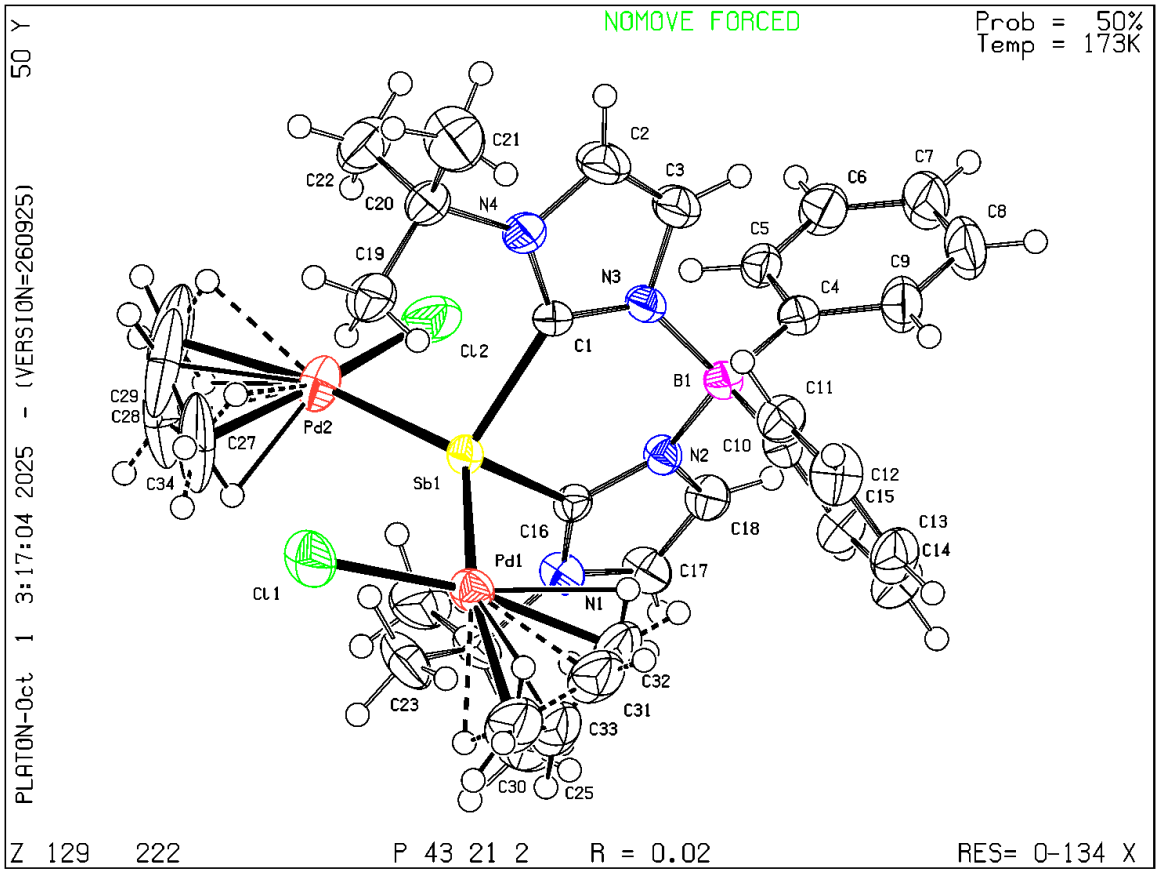
duplicate check

No duplication found

Datablock 222 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) zjy_3_502_2_auto

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: zjy_3_502_2_auto [(^{Ph,tBu}BCB)Sb(C_6F_4)BF(C_6F_5)$_2$] (**5**)

Bond precision: C-C = 0.0088 A Wavelength=1.54184

Cell: a=12.2361(3) b=13.8674(4) c=16.8994(5)
alpha=99.843(2) beta=107.396(3) gamma=105.785(2)
Temperature: 173 K

	Calculated	Reported
Volume	2531.87(14)	2531.87(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H32 B2 F15 N4 Sb, C4 H10 O [+ solvent]	C44 H32 B2 F15 N4 Sb, C4 H10 O
Sum formula	C48 H42 B2 F15 N4 O Sb [+ solvent]	C48 H42 B2 F15 N4 O Sb
Mr	1119.24	1119.22
Dx,g cm-3	1.468	1.468
Z	2	2
Mu (mm-1)	5.165	5.165
F000	1124.0	1124.0
F000'	1128.13	
h,k,lmax	15,17,21	15,17,21
Nref	10764	10216
Tmin,Tmax	0.565,0.597	0.736,1.000
Tmin'	0.072	

Correction method= # Reported T Limits: Tmin=0.736 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.949 Theta(max)= 77.597

R(reflections)= 0.0554(8583) wR2(reflections)= 0.1558(10216)

S = 1.063 Npar= 648

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 B See "Response to Alerts" below.

PLAT220_ALERT_2_B NonSolvent Resd 1 F Ueq(max)/Ueq(min) Range 7.0 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for F01Z --B1 . 19.0 s.u.
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of B1 Check

---

Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for F007 --C01B . 5.3 s.u.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C018 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O00Q 0.102 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00878 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 29 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check

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Alert level G

PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 169 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 109 Note
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= 0.600 520 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.3 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
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6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
4 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Response to Alerts:

PLAT220_ALERT_2_B (NonSolvent Resd 1 F Ueq(max)/Ueq(min) Range 7.0 Ratio):
The relatively large Ueq ratio for the peripheral fluorine atom reflects anisotropic displacement typical of terminal F atoms. The electron density is well defined, and the connectivity and geometry are unambiguous.

PLAT230_ALERT_2_B (Hirshfeld Test Diff for F01Z —B1 . 19.0 s.u.):
The high Hirshfeld rigid-bond test value arises from the light B atom bonded to highly electronegative F, which leads to differences in displacement parameters. The bond length is chemically reasonable and supported by clear electron density.

PLAT242_ALERT_2_B (Low 'MainMol' Ueq as Compared to Neighbors of B1):The lower Ueq for B1 compared to its neighbors results from scattering power differences between B and surrounding heavier atoms. The displacement parameters remain physically reasonable, and the structure is fully consistent with expected bonding.

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

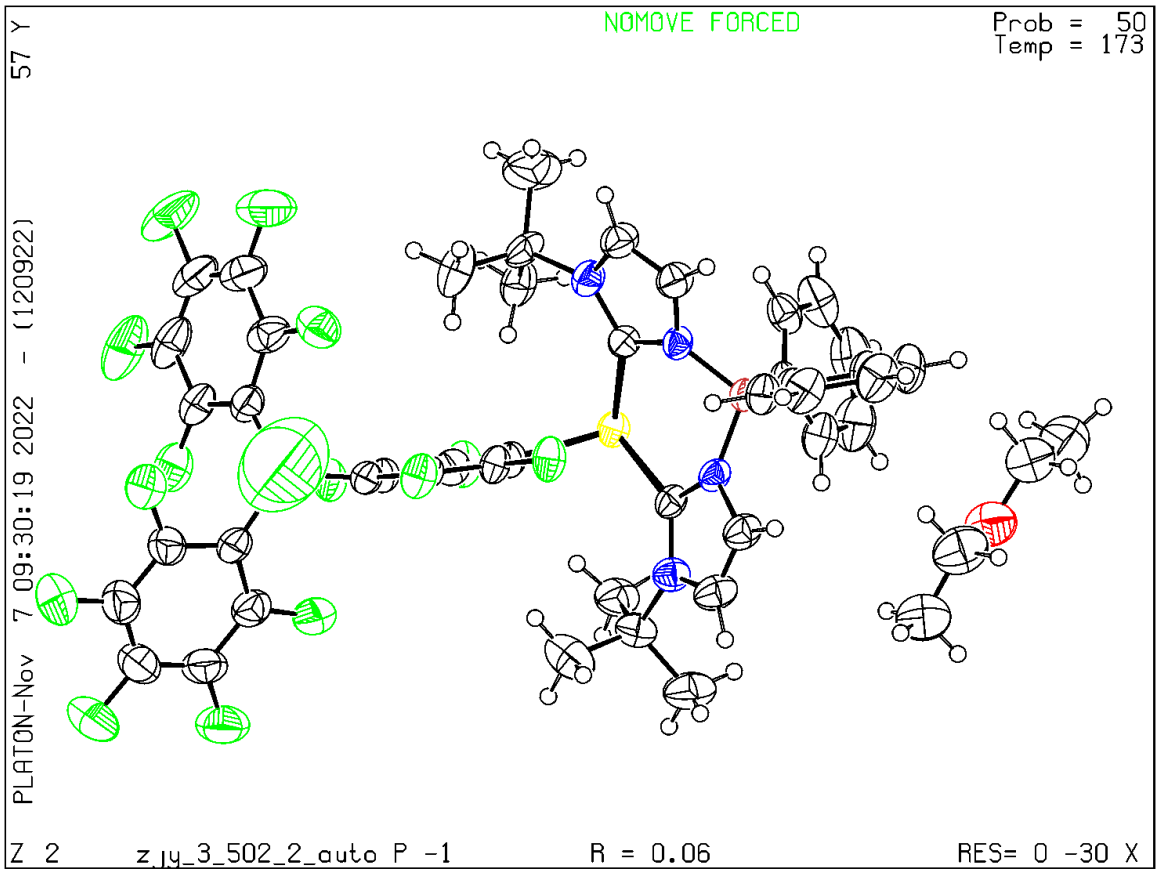
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 12/09/2022; check.def file version of 09/08/2022

Datablock zjy_3_502_2_auto - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 111

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: 111 [(^{Ph,tBu}BCB)Sb-$(CH_2)_4$-O-B$(C_6F_5)_3$] (**6**)

Bond precision: C-C = 0.0088 A Wavelength=1.54184

Cell: a=10.1787(4) b=16.4092(7) c=16.6567(7)
alpha=76.492(4) beta=85.744(3) gamma=73.440(4)
Temperature: 293 K

	Calculated	Reported
Volume	2592.8(2)	2592.8(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C48 H40 B2 F15 N4 O Sb, C4 H10 O	C48 H40 B2 F15 N4 O Sb, C4 H10 O
Sum formula	C52 H50 B2 F15 N4 O2 Sb	C52 H50 B2 F15 N4 O2 Sb
Mr	1191.34	1191.33
Dx,g cm-3	1.526	1.526
Z	2	2
Mu (mm-1)	5.096	5.096
F000	1204.0	1204.0
F000'	1208.36	
h,k,lmax	11,19,19	11,19,19
Nref	8831	8812
Tmin,Tmax	0.941,0.950	0.411,1.000
Tmin'	0.601	

Correction method= # Reported T Limits: Tmin=0.411 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 65.088

R(reflections)= 0.0659(7366) wR2(reflections)= 0.1527(8812)

S = 1.020 Npar= 693

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

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.158
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5882
PLAT213_ALERT_2_C Atom F2              has ADP max/min Ratio .....        3.2 oblate
PLAT213_ALERT_2_C Atom C11             has ADP max/min Ratio .....        3.1 oblate
PLAT213_ALERT_2_C Atom C13             has ADP max/min Ratio .....        3.1 oblate
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.6 Ratio
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00884 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     12.694 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.393 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.588         17 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.97Ang From Sb1             2.13 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.09Ang From Sb1             2.00 eA-3
```

Alert level G

```
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          2 Report
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........      0.158 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0050 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
              C4 H10 O
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          6 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        76% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         46 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.8 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  12 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or deficient
  12 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

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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 10/05/2023; check.def file version of 10/05/2023

Datablock 111 - ellipsoid plot