checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1b, 1c, 1d, 1f

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: 1b

```
Bond precision:  C-C = 0.0024 A          Wavelength=0.71075

Cell:            a=9.2417(7)    b=14.0757(10)       c=10.7643(8)
                 alpha=90       beta=110.756(1)     gamma=90
Temperature:     100 K

                Calculated                Reported
Volume          1309.38(17)               1309.38(17)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C14 H14 Cl N Pd S         C14 H14 Cl N Pd S
Sum formula     C14 H14 Cl N Pd S         C14 H14 Cl N Pd S
Mr              370.17                    370.17
Dx,g cm-3       1.878                     1.878
Z               4                         4
Mu (mm-1)       1.759                     1.759
F000            736.0                     736.0
F000'           733.26
h,k,lmax        12,18,13                  11,18,13
Nref            2993                      2991
Tmin,Tmax       0.869,0.884               0.853,1.000
Tmin'           0.869

Correction method= # Reported T Limits: Tmin=0.853 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 27.485

R(reflections)= 0.0190( 2885)     wR2(reflections)= 0.0519( 2991)

S = 1.052                  Npar= 164
```

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 G

```
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd1    --  Cl1     ..        6.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd1    --  S1      ..        5.5 s.u.
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)          2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density          8 Note
```

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

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

Datablock: 1c

```
Bond precision:  C-C = 0.0038 A          Wavelength=0.71075

Cell:            a=16.0569(8)     b=13.8191(7)     c=13.5789(7)
                 alpha=90         beta=90          gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	3013.1(3)	3013.0(3)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C15 H16 Cl N Pd S	C15 H16 Cl N Pd S
Sum formula	C15 H16 Cl N Pd S	C15 H16 Cl N Pd S
Mr	384.20	384.20
Dx,g cm-3	1.694	1.694
Z	8	8
Mu (mm-1)	1.533	1.533
F000	1536.0	1536.0
F000’	1530.54	
h,k,lmax	20,17,17	20,17,17
Nref	3468	3459
Tmin,Tmax	0.739,0.819	0.771,1.000
Tmin’	0.718	

```
Correction method= # Reported T Limits: Tmin=0.771 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 27.514

R(reflections)= 0.0268( 3353)     wR2(reflections)= 0.0691( 3459)
```

S = 1.047 Npar= 173

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

PLAT230_ALERT_2_B Hirshfeld Test Diff for C13 -- C14 .. 8.7 s.u.

Author Response: Indications of a minor disorder componant of propyl group which has not been modelled

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Alert level C

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 7 Report

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Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 6.16 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pd1 -- S1 .. 6.7 s.u.
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min) 1 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density 9 Note

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3 ALERT type 3 Indicator that the structure quality may be low
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0 ALERT type 5 Informative message, check

Datablock: 1d

Bond precision: C-C = 0.0099 A Wavelength=0.71073

Cell: a=13.4632(9) b=14.2355(10) c=17.8833(16)
alpha=90 beta=111.953(1) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	3178.9(4)	3178.9(4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C18 H14 Cl N Pd S	C18 H14 Cl N Pd S
Sum formula	C18 H14 Cl N Pd S	C18 H14 Cl N Pd S
Mr	418.21	418.21
Dx,g cm-3	1.748	1.748
Z	8	8
Mu (mm-1)	1.461	1.461
F000	1664.0	1664.0
F000’	1658.60	
h,k,lmax	17,18,23	17,18,23
Nref	7300	7260
Tmin,Tmax	0.916,0.985	0.918,0.985
Tmin’	0.916	

Correction method= # Reported T Limits: Tmin=0.918 Tmax=0.985
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 27.481

R(reflections)= 0.0586(4302) wR2(reflections)= 0.1033(7260)

S = 1.007 Npar= 397

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 ...............    0.00994 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact Cl11   ..  S1      ..       3.37 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      3.390 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min)          10 Note
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600         22 Report
PLAT977_ALERT_2_C Check the Negative Difference Density on     H14      -0.36 eA-3
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Alert level G

```
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       5.51 Why ?
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          9 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density           1 Note
```

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```
   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
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   0 ALERT type 5 Informative message, check
```

Datablock: 1f

```
Bond precision:  C-C = 0.0030 A          Wavelength=0.71075

Cell:            a=11.3879(8)     b=13.8646(10)     c=21.6304(15)
                 alpha=90         beta=90           gamma=90
Temperature:     100 K

                Calculated                Reported
Volume          3415.2(4)                 3415.2(4)
Space group     P b c a                   P b c a
Hall group      -P 2ac 2ab                -P 2ac 2ab
Moiety formula  C19 H16 Cl N O Pd S       C19 H16 Cl N O Pd S
Sum formula     C19 H16 Cl N O Pd S       C19 H16 Cl1 N1 O1 Pd1 S1
Mr              448.24                    448.25
Dx,g cm-3       1.744                     1.744
Z               8                         8
Mu (mm-1)       1.370                     1.370
F000            1792.0                    1792.0
F000'           1786.69
h,k,lmax        14,18,28                  14,18,28
Nref            3918                      3916
Tmin,Tmax       0.835,0.960               0.796,1.000
Tmin'           0.825

Correction method= # Reported T Limits: Tmin=0.796 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 27.484

R(reflections)= 0.0229( 3343)     wR2(reflections)= 0.0604( 3916)

S = 1.064                  Npar= 218
```

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 G

```
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)          1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density          7 Note
```

```
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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

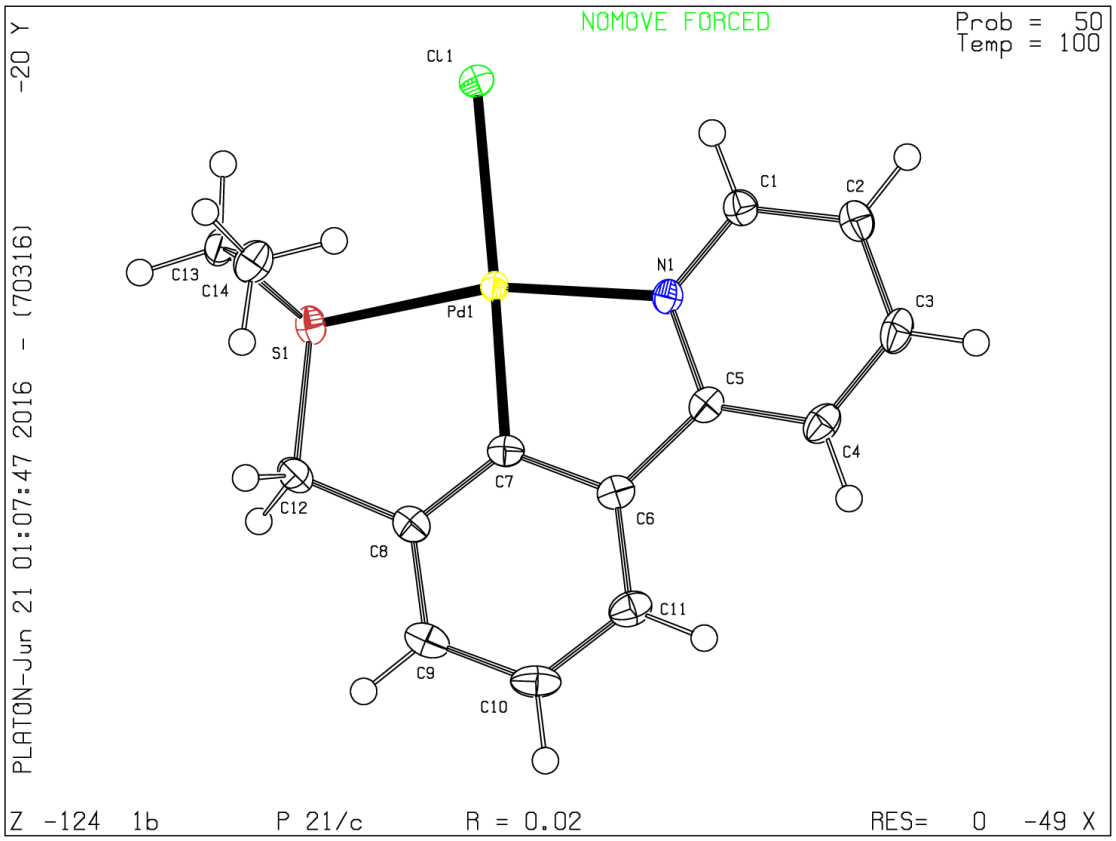
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

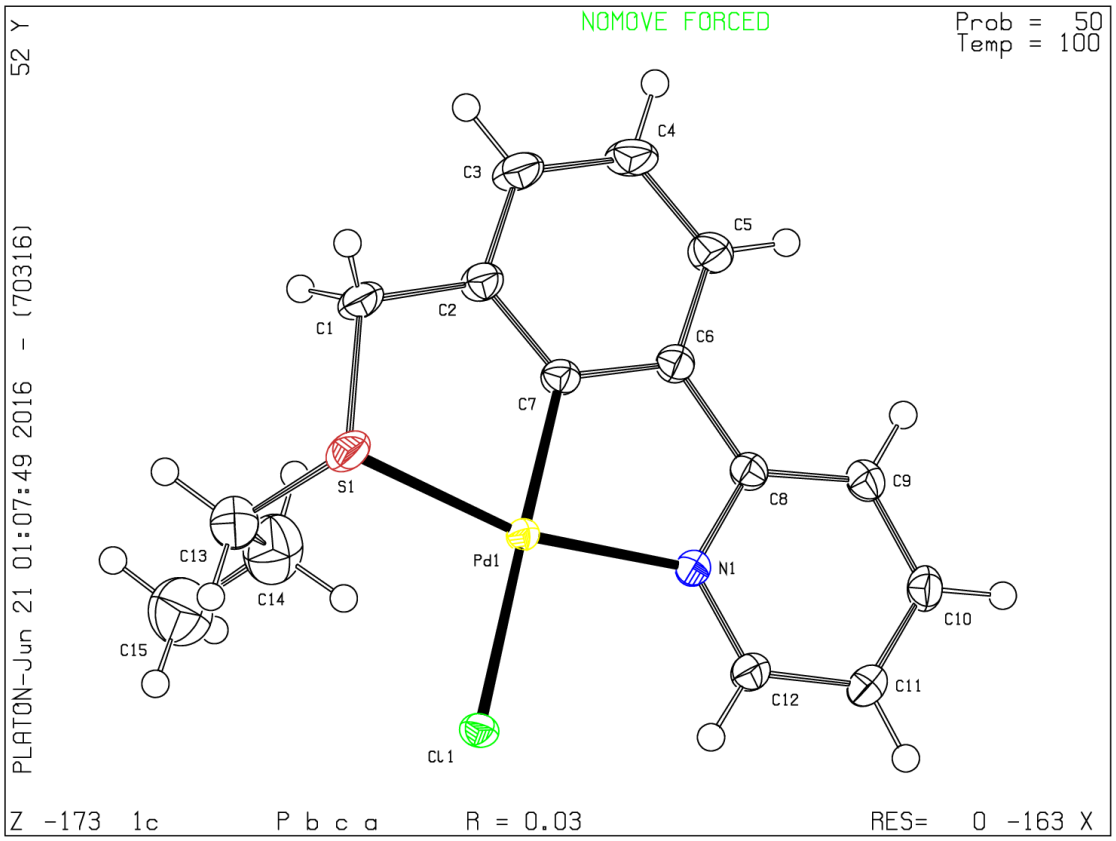
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 06/05/2016; check.def file version of 05/05/2016

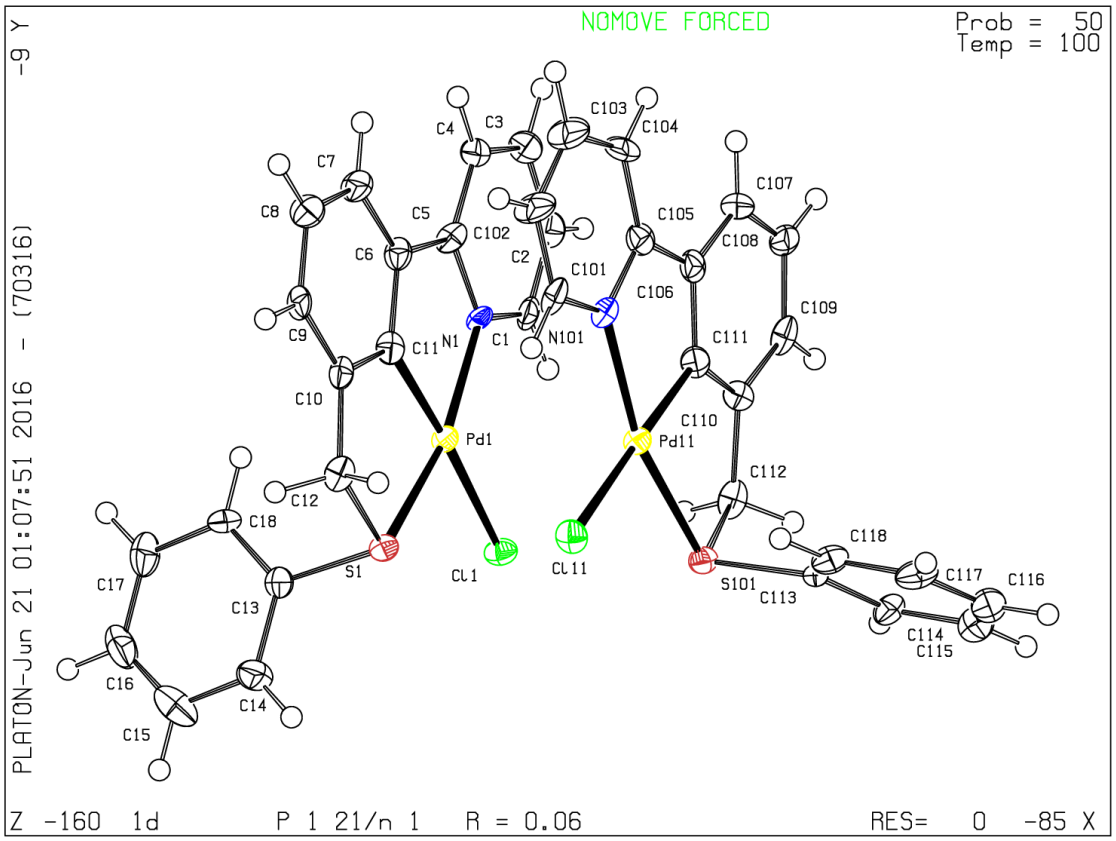
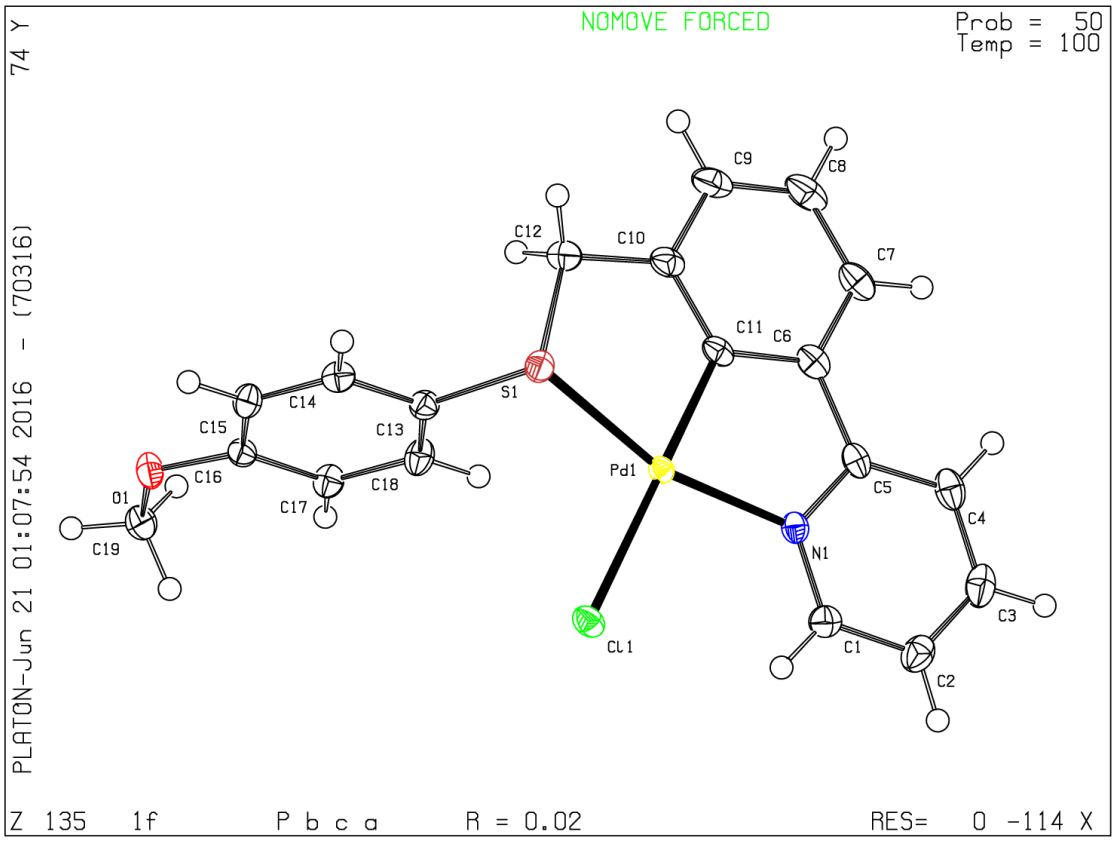
Datablock 1b - ellipsoid plot



Datablock 1c - ellipsoid plot



Datablock 1d - ellipsoid plot



Datablock 1f - ellipsoid plot