checkCIF/PLATON report

Structure factors have been supplied for datablock(s) pttdtn_0m

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: pttdtn_0m

```
Bond precision:  C-C = 0.0093 A          Wavelength=0.71073

Cell:          a=8.9894(3)        b=9.0013(3)      c=11.4059(4)
               alpha=101.627(2)   beta=90.517(2)   gamma=110.844(2)
Temperature:   173 K
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	Calculated	Reported
Volume	841.53(5)	841.53(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C12 H11 Cl4 N3 Pt S2	C12 H11 Cl2 N3 Pt1 S2
Sum formula	C12 H11 Cl4 N3 Pt S2	C12 H11 Cl4 N3 Pt S2
Mr	598.24	598.25
Dx,g cm-3	2.361	2.361
Z	2	2
Mu (mm-1)	9.216	9.216
F000	564.0	564.0
F000’	562.56	
h,k,lmax	12,12,15	12,12,15
Nref	4211	4166
Tmin,Tmax	0.081,0.331	0.355,0.746
Tmin’	0.015	

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Correction method= # Reported T Limits: Tmin=0.355 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.989          Theta(max)= 28.383

R(reflections)= 0.0248( 4079)     wR2(reflections)= 0.0912( 4166)

S = 1.570                 Npar= 199
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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 B

```
PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ...          3 Check
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....          3 Check
PLAT939_ALERT_3_B Large Value of Not (SHELXL) Weight Optimized S .     486.69 Check
PLAT972_ALERT_2_B Check Calcd Resid. Dens.  0.96A   From Pt             -2.67 eA-3
```

Alert level C

```
PLAT213_ALERT_2_C Atom Cl3             has ADP max/min Ratio .....        3.1 prolat
PLAT220_ALERT_2_C Non-Solvent  Resd 1 Cl   Ueq(max)/Ueq(min) Range        3.5 Ratio
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00925 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact  Cl4      ..S2       .       3.42 Ang.
                                          -1-x,1-y,2-z  =      2_467 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          9 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          3 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.88A   From Pt              1.99 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.44A   From C11             1.99 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.73A   From Pt              1.84 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.10A   From Cl4             1.55 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.86A   From Pt             -2.10 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.91A   From Pt             -2.09 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.94A   From Pt             -1.77 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2A              -0.64 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2B              -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H12              -0.50 eA-3
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C12 H11 Cl4 N3 Pt1 S2
           Atom count from _chemical_formula_moiety:C12 H11 Cl2 N3 Pt1 S2
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.002 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl2      ..C1               3.19 Ang.
                                          -x,1-y,1-z  =      2_566 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pt        (II)      .       2.15 Info
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         37 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          4 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
  16 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   8 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  16 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 pttdtn_0m - ellipsoid plot