checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: TM-PDS-STP

```
Bond precision:  C-C = 0.0096 A          Wavelength=0.71070

Cell:            a=5.2296(10)     b=11.006(2)        c=31.718(6)
                 alpha=90         beta=93.903(6)     gamma=90
Temperature:     293 K
```

	Calculated	Reported
Volume	1821.4(6)	1821.4(6)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	?
Moiety formula	C14 H10 O S4 Se4	?
Sum formula	C14 H10 O S4 Se4	C14 H10 O S4 Se4
Mr	638.34	638.30
Dx,g cm-3	2.328	2.328
Z	4	4
Mu (mm-1)	8.514	8.514
F000	1208.0	1208.0
F000’	1209.09	
h,k,lmax	6,14,41	6,14,41
Nref	4180	4129
Tmin,Tmax	0.374,0.653	0.281,0.675
Tmin’	0.175	

```
Correction method= MULTI-SCAN

Data completeness= 0.988          Theta(max)= 27.480

R(reflections)= 0.0601( 2787)     wR2(reflections)= 0.1596( 4129)

S = 1.068                 Npar= 211
```

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

```
PLAT048_ALERT_1_C MoietyFormula Not Given .....................        ?
PLAT125_ALERT_4_C No ’_symmetry_space_group_name_Hall’ Given .....        ?
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.0096 Ang
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c   .......      P21/n
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature        293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature        293 K
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **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

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

Datablock: TM-PDS-STP_PF6_PhCl

Bond precision: C-C = 0.0133 A Wavelength=0.71070

Cell: a=7.917(3) b=10.582(3) c=15.979(5)
alpha=76.666(16) beta=89.916(17) gamma=89.124(19)
Temperature: 293 K

	Calculated	Reported
Volume	1302.4(7)	1302.5(7)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	2(C14 H10 O S4 Se4), 2(F6 P), C6 H5 Cl	?
Sum formula	C34 H25 Cl F12 O2 P2 S8 Se8	C17 H12.50 Cl0.50 F6 O P S4 Se4
Mr	1679.17	839.54
Dx,g cm-3	2.141	2.141
Z	1	2
Mu (mm-1)	6.121	6.121
F000	800.0	800.0
F000’	801.05	
h,k,lmax	10,13,20	10,13,20
Nref	5974	5841
Tmin,Tmax	0.485,0.941	0.206,0.294
Tmin’	0.291	

Correction method= MULTI-SCAN

Data completeness= 0.978 Theta(max)= 27.480

R(reflections)= 0.0786(2799) wR2(reflections)= 0.2846(5841)

S = 0.964 Npar= 382

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

PLAT234_ALERT_4_B Large Hirshfeld Difference P1 -- F3B .. 0.30 Ang.

Alert level C

RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25
Weighted R factor given 0.285
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low .... 48 Perc.
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.977
PLAT045_ALERT_1_C Calculated and Reported Z Differ by ..... 0.50 Ratio
PLAT048_ALERT_1_C MoietyFormula Not Given ..... ?
PLAT084_ALERT_2_C High wR2 Value 0.28
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.92
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given ..... ?
PLAT234_ALERT_4_C Large Hirshfeld Difference S4 -- C14 .. 0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C11 -- C12 .. 0.17 Ang.
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for O1
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of P1
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.3
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0133 Ang

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 18
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites 12
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms 2
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.17
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature 293 K
PLAT200_ALERT_1_G Check the Reported _diffrn_ambient_temperature 293 K
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ..... 71 Perc.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 77
F6B -P1 -F5A 1.555 1.555 1.555 40.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 84
F5B -P1 -F4A 1.555 1.555 1.555 40.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 89
F3A -P1 -F4B 1.555 1.555 1.555 39.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 108
CL1 -C15 -H15 1.555 1.555 1.555 8.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 114
CL2 -C16 -H16 1.555 1.555 1.555 7.70 Deg.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... !
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 181

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```
   4 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
   5 ALERT type 3 Indicator that the structure quality may be low
  11 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
```

Datablock: TM-TPDS-STP_PF6_PhCl

Bond precision: C-C = 0.0147 A Wavelength=0.71070

Cell: a=12.666(3) b=14.299(4) c=16.289(5)
       alpha=85.39(2) beta=88.219(19) gamma=79.788(18)
Temperature: 293 K

	Calculated	Reported
Volume	2893.6(14)	2893.6(14)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	2(C14 H10 S5 Se4), 0.5(C12 H10.02 Cl2), C6 H5 Cl, 2(F6 P)	?
Sum formula	C40 H30 Cl2 F12 P2 S10 Se8	C40 H30 Cl2 F12 P2 S10 Se8
Mr	1823.83	1823.76
Dx,g cm-3	2.093	2.093
Z	2	2
Mu (mm-1)	5.631	5.631
F000	1748.0	1748.0
F000’	1750.84	
h,k,lmax	16,18,21	16,18,21
Nref	13248	12916
Tmin,Tmax	0.588,0.945	0.192,0.324
Tmin’	0.425	

Correction method= MULTI-SCAN

Data completeness= 0.975 Theta(max)= 27.460

R(reflections)= 0.0745(6484) wR2(reflections)= 0.2674(12916)

S = 0.974 Npar= 689

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

PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for S9

```
PLAT366_ALERT_2_B Short? C(sp?)-C(sp?) Bond  C36    -   C37    ...       1.27 Ang.
PLAT431_ALERT_2_B Short Inter HL..A  Contact  F3     ..  Cl3     .       2.77 Ang.
```

Alert level C

```
RFACR01_ALERT_3_C  The value of the weighted R factor is > 0.25
           Weighted R factor given   0.267
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......      0.975
PLAT048_ALERT_1_C MoietyFormula Not Given ........................         ?
PLAT084_ALERT_2_C High wR2 Value .................................      0.27
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given .....         ?
PLAT220_ALERT_2_C Large Non-Solvent    C     Ueq(max)/Ueq(min) ...       3.2 Ratio
PLAT220_ALERT_2_C Large Non-Solvent    S     Ueq(max)/Ueq(min) ...       3.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C25    --  C26     ..      0.16 Ang.
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       S10
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C25
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C38
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C40
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors of        C31
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors of        C33
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        C29
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        C32
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        C34
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         P1
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         P2
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.0147 Ang
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond  C35    -   C40    ...       1.34 Ang.
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond  C37    -   C38    ...       1.31 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  F6     ..  Cl4     .       3.12 Ang.
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C40 H30 Cl2 F12 P2 S10 Se8
           Atom count from the _atom_site data:  C40 H30.01 Cl1.99 F12 P2 S10 S
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         16
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....         16
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.15
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature       293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature       293 K
PLAT301_ALERT_3_G Note: Main Residue  Disorder ..................          3 Perc.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C31    ..  Cl3     ..      3.03 Ang.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......       265
```

```
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   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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   9 ALERT type 4 Improvement, methodology, query or suggestion
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```

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checkCIF publication errors

Alert level A

```
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
            Abstract of paper in English.
```

Alert level G

```
PUBL013_ALERT_1_G The _publ_section_comment (discussion of study) is
            missing. This is required for a full paper submission (but is
            optional for an electronic paper).
PUBL017_ALERT_1_G The _publ_section_references section is missing or
            empty.
```

2 **ALERT level A** = Data missing that is essential or data in wrong format
2 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.

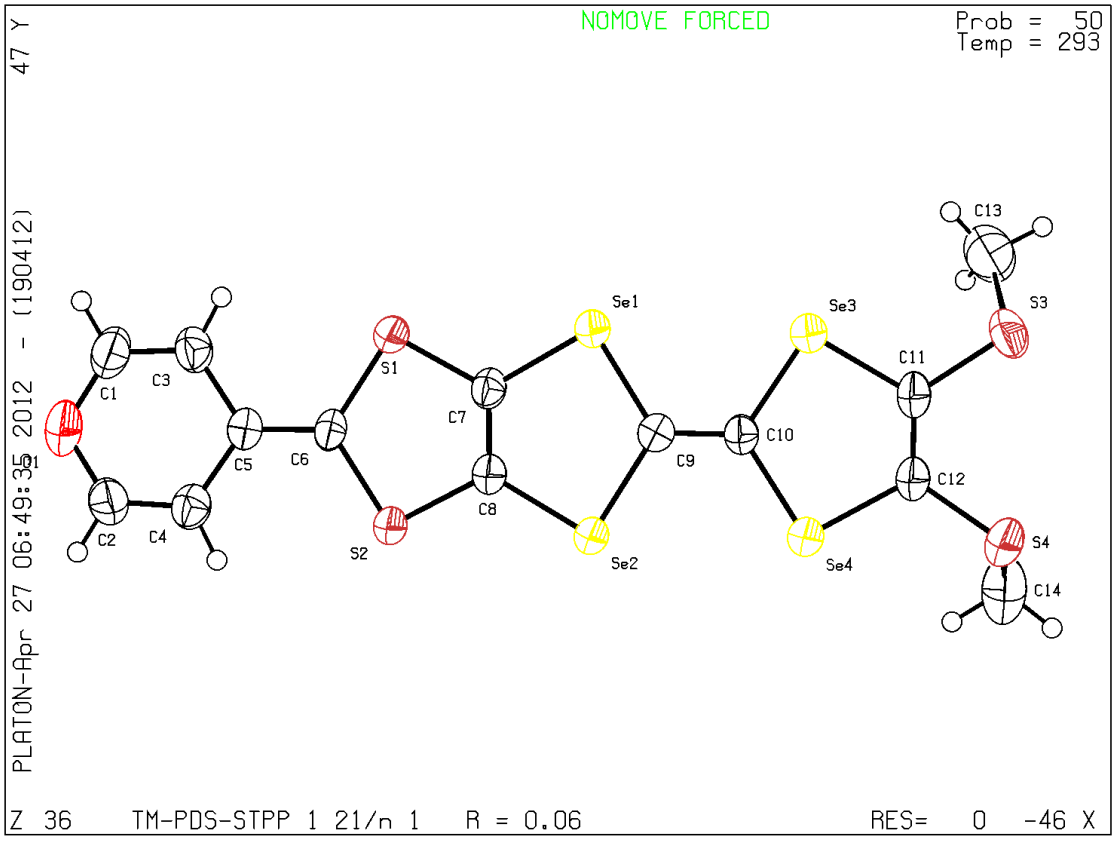
If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.

```
# start Validation Reply Form
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

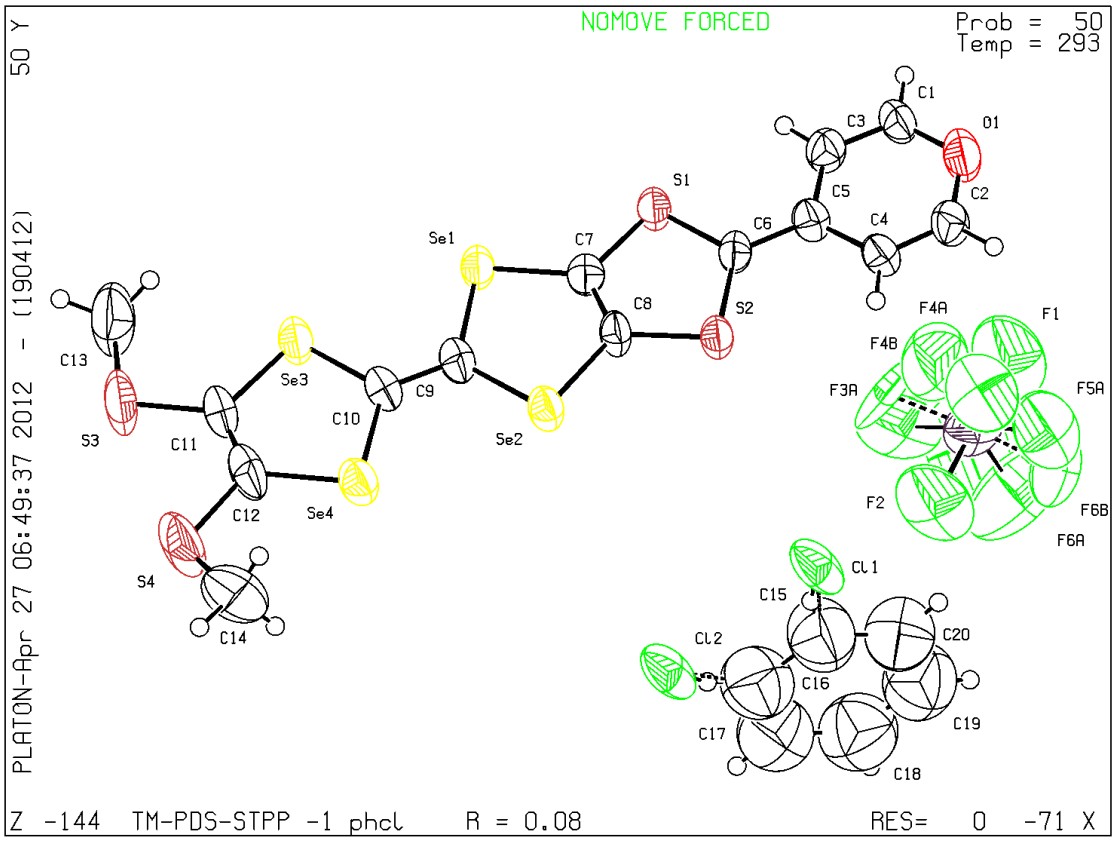
If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 19/04/2012; check.def file version of 14/04/2012

Datablock TM-PDS-STP - ellipsoid plot



Datablock TM-PDS-STP_PF6_PhCl - ellipsoid plot



Datablock TM-TPDS-STP_PF6_PhCl - ellipsoid plot