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

Bond precision: C-C = 0.0336 A Wavelength=1.54180

Cell: a=11.9727(9) b=12.3610(9) c=12.8053(10)
alpha=66.932(7) beta=62.152(8) gamma=63.125(7)
Temperature: 150 K

	Calculated	Reported
Volume	1454.9(2)	1454.9(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C54 H72 N4 S2, 2(C F3 O3 S)	C27 H36 N2 S, C F3 O3 S
Sum formula	C56 H72 F6 N4 O6 S4	C28 H36 F3 N2 O3 S2
Mr	1139.42	569.74
Dx,g cm-3	1.301	1.300
Z	1	2
Mu (mm-1)	2.094	2.094
F000	602.0	605.2
F000’	605.13	
h,k,lmax	14,15,15	14,15,15
Nref	5752	4780
Tmin,Tmax	0.720,0.778	0.456,1.000
Tmin’	0.653	

Correction method= MULTI-SCAN

Data completeness= 0.831 Theta(max)= 72.420

R(reflections)= 0.3194(2536) wR2(reflections)= 0.7521(4780)

S = 3.400 Npar= 350

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 A

```
RFACG01_ALERT_3_A  The value of the R factor is > 0.20
           R factor given   0.319
RFACR01_ALERT_3_A  The value of the weighted R factor is > 0.45
           Weighted R factor given   0.752
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low .......      0.831 Note
PLAT082_ALERT_2_A High R1 Value ..................................       0.32 Report
PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ...................       0.75 Report
PLAT234_ALERT_4_A Large Hirshfeld Difference C2     --  C3      ..       0.32 Ang.
```

Alert level B

```
DIFMN02_ALERT_2_B  The minimum difference density is < -0.1*ZMAX*1.00
           _refine_diff_density_min given =     -2.493
           Test value =     -1.600
DIFMX01_ALERT_2_B  The maximum difference density is > 0.1*ZMAX*1.00
           _refine_diff_density_max given =      2.750
           Test value =      1.600
SHFSU01_ALERT_2_B  The absolute value of parameter shift to su ratio > 0.10
           Absolute value of the parameter shift to su ratio given   0.157
           Additional refinement cycles may be required.
PLAT080_ALERT_2_B Maximum Shift/Error ............................       0.16
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density      2.75 eA-3
PLAT098_ALERT_2_B Large Reported Min.  (Negative) Residual Density     -2.49 eA-3
PLAT234_ALERT_4_B Large Hirshfeld Difference F3     --  C28     ..       0.28 Ang.
PLAT242_ALERT_2_B Low       Ueq as Compared to Neighbors for .....        C13 Check
PLAT340_ALERT_3_B Low Bond Precision on  C-C Bonds ...............     0.0336 Ang.
```

Alert level C

```
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
           The relevant atom site should be identified.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
GOODF01_ALERT_2_C  The least squares goodness of fit parameter lies
           outside the range 0.80 <> 2.00
           Goodness of fit given =      3.400
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT087_ALERT_2_C Unsatisfactory S value (Too High) ..............       3.40 Check
PLAT234_ALERT_4_C Large Hirshfeld Difference N2     --  C3      ..       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C17    --  C18     ..       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference S2     --  O1      ..       0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference S2     --  O3      ..       0.18 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....         C3 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C10 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C20 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C19 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C25 Check
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors of         C28 Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of          S2 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....       3.7 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....       2.8 Note
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C13    -   C14    ...      1.43 Ang.
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ............       0.50 Ratio
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.20 Report
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   F2     --  C28     ..        6.0 su
```

```
PLAT333_ALERT_2_G Check Large Av C6-Ring C-C Dist. C16    -C21          1.42 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact  F1     ..  F1      .       2.70 Ang.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         2 Note
             C F3 O3 S
PLAT982_ALERT_1_G The  C-f'=     0.019 Deviates from the  IT-value      0.018 Check
PLAT982_ALERT_1_G The  F-f'=     0.075 Deviates from the  IT-value      0.073 Check
PLAT982_ALERT_1_G The  N-f'=     0.033 Deviates from the  IT-value      0.031 Check
PLAT982_ALERT_1_G The  O-f'=     0.052 Deviates from the  IT-value      0.049 Check
PLAT982_ALERT_1_G The  S-f'=     0.335 Deviates from the  IT-value      0.333 Check
```

```
   6 ALERT level A = Most likely a serious problem - resolve or explain
   9 ALERT level B = A potentially serious problem, consider carefully
  19 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

  10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  21 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
  10 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*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

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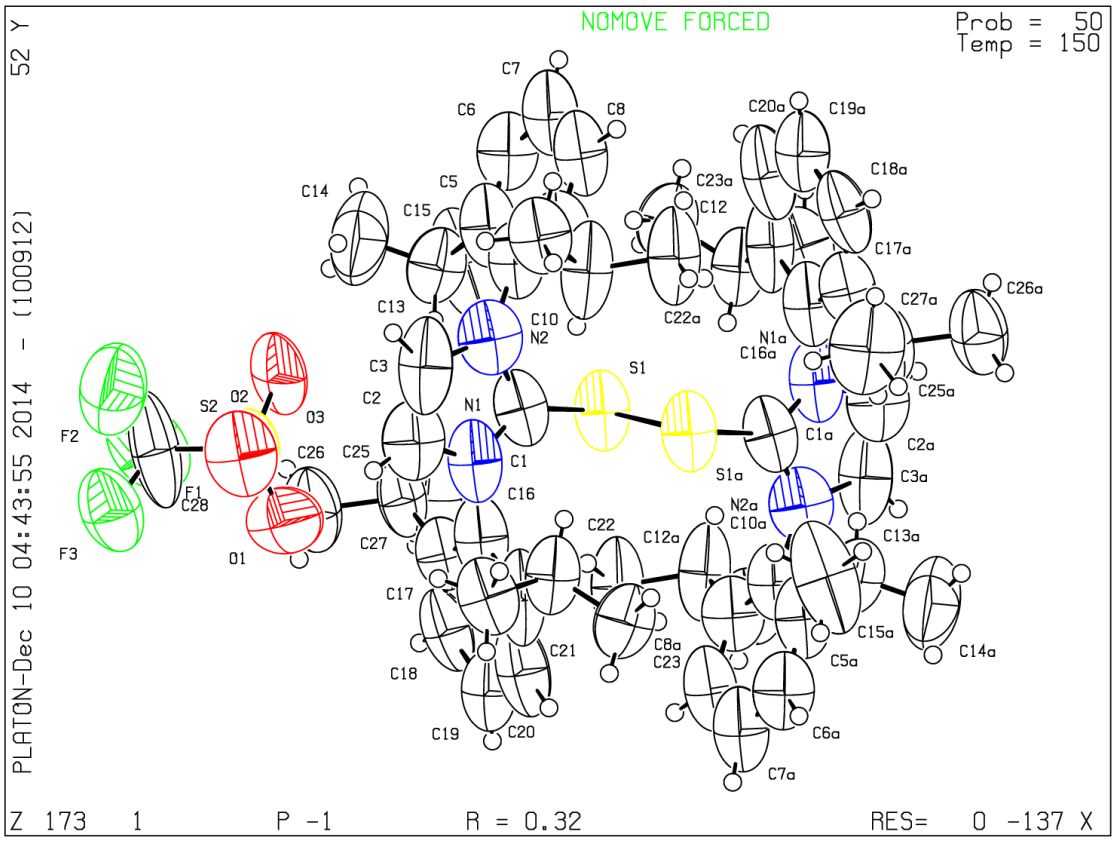
PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock 1 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 2

Bond precision: C-C = 0.0038 A Wavelength=1.54180

Cell: a=11.7507(8) b=12.2346(8) c=12.6554(8)
alpha=89.826(5) beta=64.316(7) gamma=65.087(7)
Temperature: 150 K

	Calculated	Reported
Volume	1450.8(2)	1450.74(17)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C54 H72 N4 Se2, 2(C F3 O3 S)	C54 H72 N4 Se2, 2(C F3 O3 S)
Sum formula	C56 H72 F6 N4 O6 S2 Se2	C56 H72 F6 N4 O6 S2 Se2
Mr	1233.22	1233.22
Dx,g cm-3	1.411	1.412
Z	1	1
Mu (mm-1)	2.862	2.862
F000	638.0	638.0
F000’	638.86	
h,k,lmax	14,14,15	14,14,15
Nref	5592	5461
Tmin,Tmax	0.627,0.709	0.954,1.000
Tmin’	0.537	

Correction method= MULTI-SCAN

Data completeness= 0.977 Theta(max)= 70.770

R(reflections)= 0.0336(4878) wR2(reflections)= 0.0859(5461)

S = 1.022 Npar= 351

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

```
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......      0.977 Note
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        3.5 Ratio
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C10 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C22 Check
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .      mixed
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...          3 Units
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of         C28 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact  F3     ..  F3      .       2.83 Ang.
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
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   2 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
   1 ALERT type 3 Indicator that the structure quality may be low
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   1 ALERT type 5 Informative message, check
```

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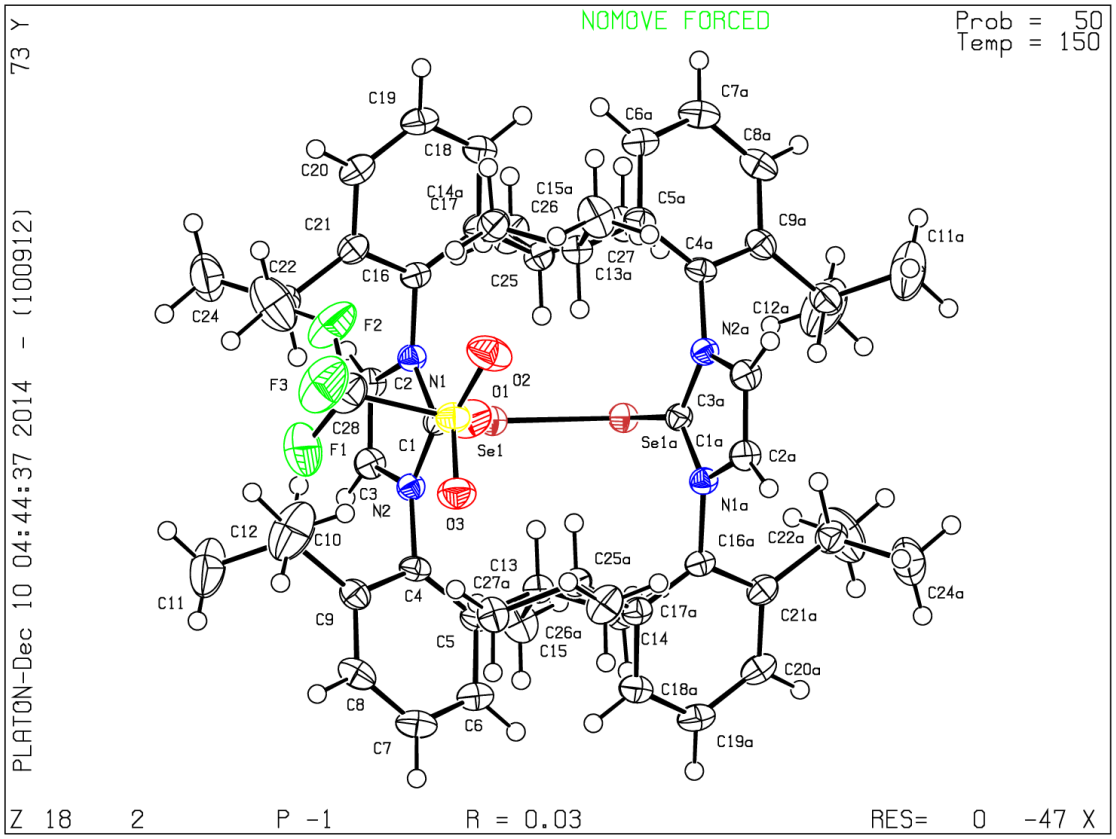
Datablock 2 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3

Bond precision: C-C = 0.0111 A Wavelength=0.71070

Cell: a=13.3074(3) b=18.1568(3) c=18.3035(3)
alpha=90 beta=90 gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	4422.49(14)	4422.51(13)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C36 H48 N4 O4 Se2, 2(Cl O4), C H4 O	C36 H48 N4 O4 Se2, 2(Cl O4), C H4 O
Sum formula	C37 H52 Cl2 N4 O13 Se2	C37 H52 Cl2 N4 O13 Se2
Mr	989.65	989.67
Dx,g cm-3	1.486	1.486
Z	4	4
Mu (mm-1)	1.857	1.857
F000	2032.0	2033.5
F000’	2033.34	
h,k,lmax	18,24,25	17,24,23
Nref	11848[6506]	9590
Tmin,Tmax	0.895,0.928	0.897,1.000
Tmin’	0.862	

Correction method= MULTI-SCAN

Data completeness= 1.47/0.81 Theta(max)= 29.090

R(reflections)= 0.0651(8380) wR2(reflections)= 0.1706(9590)

S = 1.032 Npar= 536

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 A

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low ..... 0.810 Note
PLAT430_ALERT_2_A Short Inter D...A Contact Se1 .. O5 .. 2.88 Ang.

Alert level C

STRVA01_ALERT_2_C Chirality of atom sites is inverted?
From the CIF: _refine_ls_abs_structure_Flack 0.983
From the CIF: _refine_ls_abs_structure_Flack_su 0.007
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C13 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0111 Ang.

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT033_ALERT_4_G Flack x Value Deviates > 2*sigma from Zero 0.983
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 20.13 Why ?
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 33 Note
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of Cl1 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of Cl2 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O8 .. C23 .. 2.91 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact O9 .. C19 .. 2.93 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact O9 .. C23 .. 2.98 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact O12 .. C2 .. 3.02 Ang.
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ 2 Units
PLAT982_ALERT_1_G The Se-f'= -0.081 Deviates from the IT-value -0.093 Check
PLAT983_ALERT_1_G The Se-f"= 2.308 Deviates from the IT-Value 2.226 Check

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Datablock 3 - ellipsoid plot