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 Å  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

Volume  Calculated  Reported  
        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_3_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
**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
**PLAT242_ALERT_2_C**  Low 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
| ALERT level A | Most likely a serious problem – resolve or explain |
| ALERT level B | A potentially serious problem, consider carefully |
| ALERT level C | Check. Ensure it is not caused by an omission or oversight |
| 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
10 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.

**Publication of your CIF in other journals**

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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:  
\begin{align*}
a &= 11.7507(8) \\
b &= 12.2346(8) \\
c &= 12.6554(8) \\
\alpha &= 89.826(5) \\
\beta &= 64.316(7) \\
\gamma &= 65.087(7) \\
\end{align*}

Temperature:  150 K

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<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>1450.8(2)</td>
</tr>
<tr>
<td>Space group</td>
<td>P -1</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 1</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C54 H72 N4 Se2, 2(C F3 O3 S)</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C56 H72 F6 N4 O6 S2 Se2</td>
</tr>
<tr>
<td>Mr</td>
<td>1233.22</td>
</tr>
<tr>
<td>Dx, g cm(^{-3})</td>
<td>1.411</td>
</tr>
<tr>
<td>Z</td>
<td>1</td>
</tr>
<tr>
<td>Mu (mm(^{-1}))</td>
<td>2.862</td>
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<tr>
<td>F000</td>
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<td>F000(^\prime)</td>
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<tr>
<td>Tmin(^\prime)</td>
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</table>

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 

\text{test-name}_\text{ALERT}_\text{alert-type}_\text{alert-level}.

Click on the hyperlinks for more details of the test.
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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 Å  Wavelength=0.7107 Å

Cell:

\[
\begin{align*}
\text{a} &= 13.3074(3) \\
\text{b} &= 18.1568(3) \\
\text{c} &= 18.3035(3) \\
\text{alpha} &= 90 \\
\text{beta} &= 90 \\
\text{gamma} &= 90
\end{align*}
\]

Temperature: 150 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>4422.49(14)</td>
</tr>
<tr>
<td>Space group</td>
<td>P 21 21 21</td>
</tr>
<tr>
<td>Hall group</td>
<td>P 2ac 2ab</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C36 H48 N4 O4 Se2, 2(Cl O4), C H4 O</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C37 H52 Cl2 N4 O13 Se2</td>
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<td>Mr</td>
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<tr>
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<tr>
<td>Mu (mm(^{-1}))</td>
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<tr>
<td>F000</td>
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<td>18,24,25</td>
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<tr>
<td>Nref</td>
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<td>Tmin,Tmax</td>
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<tr>
<td>Tmin'</td>
<td>0.862</td>
</tr>
</tbody>
</table>

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 Sel .. 05 .. 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 C11 Check

**PLAT244_ALERT_4_G** Low ‘Solvent’ Ueq as Compared to Neighbors of C12 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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