checkCIF/PLATON report

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

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: k1_100

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Bond precision:  C-C = 0.0090 A          Wavelength=0.71070

Cell:          a=8.0239(4)       b=9.3028(5)      c=17.393(1)
               alpha=96.935(5)   beta=97.999(5)   gamma=110.093(5)
Temperature:   100 K
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	Calculated	Reported
Volume	1187.42(12)	1187.41(11)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	3(C10 H8 S8), 2(F4 Re)	?
Sum formula	C30 H24 F8 Re2 S24	C15 H12 F4 Re S12
Mr	1678.35	839.17
Dx,g cm-3	2.347	2.347
Z	1	2
Mu (mm-1)	6.210	6.210
F000	810.0	810.0
F000’	811.25	
h,k,lmax	10,12,23	10,12,23
Nref	6344	6338
Tmin,Tmax	0.599,0.733	0.373,1.000
Tmin’	0.390	

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Correction method= # Reported T Limits: Tmin=0.373 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 29.070

R(reflections)= 0.0477( 5189)     wR2(reflections)= 0.1099( 6338)

S = 1.065                 Npar= 302
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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 C

```
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.6 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference Re1      --F3'      .       0.17 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C10 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         S5 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        Re1 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.6 Note
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............      0.009 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C5       - C6       .       1.43 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C9       - C10      .       1.41 Ang.
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          7 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          6 Report
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as      mixed Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.005 Degree
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)    Re1      --F2       .        5.7 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)    Re1      --F4       .        8.5 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)    Re1      --F2'      .        5.3 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)    Re1      --F4'      .       10.5 s.u.
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )        80% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  S9       ..C7             3.30 Ang.
                                                     x,y,z  =      1_555 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
            C10 H8 S8
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
            F4 Re
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         42 Note
PLAT899_ALERT_4_G SHELXL97  is Deprecated and Succeeded by SHELXL/       2018 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  16 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 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
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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 18/09/2020; check.def file version of 20/08/2020

Datablock k1_100 - ellipsoid plot