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: 1

Bond precision: C-C = 0.0073 A Wavelength=0.71073

Cell: a=8.802(2) b=40.985(9) c=12.128(3)
alpha=90 beta=100.660(4) gamma=90
Temperature: 291 K

	Calculated	Reported
Volume	4299.7(17)	4299.7(17)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	?
Moiety formula	C36 H24 N6 Ru S4, 2(F6 P), C2 H3 N	?
Sum formula	C38 H27 F12 N7 P2 Ru S4	C38 H27 F12 N7 P2 Ru S4
Mr	1100.96	1100.92
Dx,g cm-3	1.701	1.701
Z	4	4
Mu (mm-1)	0.725	0.725
F000	2200.0	2200.0
F000’	2198.94	
h,k,lmax	10,50,14	10,50,14
Nref	8435	8321
Tmin,Tmax	0.816,0.853	0.823,0.857
Tmin’	0.816	

Correction method= MULTI-SCAN

Data completeness= 0.986 Theta(max)= 26.000

R(reflections)= 0.0539(5206) wR2(reflections)= 0.1354(8321)

S = 1.063 Npar= Npar = 578

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 G

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PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .       mixed
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of          P1 Check
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of          P2 Check
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        102 Do !
            C6  -N2  -RU1 -N5    -57.00  7.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        103 Do !
            C10 -N2  -RU1 -N5    126.00  7.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        112 Do !
            C21 -N5  -RU1 -N2    143.00  7.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        113 Do !
            C22 -N5  -RU1 -N2    -35.00  7.00   1.555   1.555   1.555   1.555
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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
   0 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   9 ALERT level G = General information/check it is not something unexpected

   2 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
   0 ALERT type 3 Indicator that the structure quality may be low
   6 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*, 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 05/02/2014; check.def file version of 05/02/2014

Datablock 1 - ellipsoid plot