

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: oz2

Bond precision: C-C = 0.0118 A Wavelength=0.71073

Cell: a=12.529(2) b=12.734(2) c=18.789(3)
 alpha=89.976(2) beta=89.898(3) gamma=89.418(2)

Temperature: 120 K

	Calculated	Reported
Volume	2997.5(8)	2997.4(8)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C25 H24 N6 Ru, 2(F6 P)	?
Sum formula	C25 H24 F12 N6 P2 Ru	C25 H24 F12 N6 P2 Ru
Mr	799.51	799.51
Dx,g cm-3	1.772	1.772
Z	4	4
Mu (mm-1)	0.734	0.734
F000	1592.0	1592.0
F000'	1588.81	
h,k,lmax	15,16,23	15,16,23
Nref	12504	12077
Tmin,Tmax	0.900,0.929	0.838,0.930
Tmin'	0.832	

Correction method= MULTI-SCAN

Data completeness= 0.966 Theta(max)= 26.550

R(reflections)= 0.0669(6076) wR2(reflections)= 0.1489(12077)

S = 0.949 Npar= 831

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 _diffn_measured_fraction_theta_full	Low	0.966
PLAT234_ALERT_4_C Large Hirshfeld Difference N6	-- C24 ..	0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C24	-- C25 ..	0.16 Ang.
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
PLAT244_ALERT_4_C Low	'Solvent' Ueq as Compared to Neighbors of	P3
PLAT244_ALERT_4_C Low	'Solvent' Ueq as Compared to Neighbors of	P4
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor		2.1
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor		2.1
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor		2.2
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds		0.0118 Ang

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF	?
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .	mixed
PLAT104_ALERT_1_G The Reported Crystal System is Inconsistent with	P-1
PLAT112_ALERT_2_G ADDSYM Detects Additional (Pseudo) Symm. Elem...	n
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space-group.	P21/c
PLAT194_ALERT_1_G Missing _cell_measurement_reflms_used datum	?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max datum	?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min datum	?
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	1
N6 -RU1 -N1 -C18 -138.00 8.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	6
N6 -RU1 -N1 -C12 99.00 8.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	11
N6 -RU1 -N1 -C1 -17.00 8.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	56
N1 -RU1 -N6 -C24 -8.00 13.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	57
N5 -RU1 -N6 -C24 -162.00 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 ... #	58
N4 -RU1 -N6 -C24 109.00 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 ... #	59
N2 -RU1 -N6 -C24 -69.00 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 ... #	60
N3 -RU1 -N6 -C24 16.00 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 ... #	61
N12 -RU2 -N7 -C37 143.00 8.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	66
N12 -RU2 -N7 -C43 -93.00 8.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	71
N12 -RU2 -N7 -C26 25.00 8.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	116
N7 -RU2 -N12 -C49 -6.00 12.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	117
N8 -RU2 -N12 -C49 -24.00 6.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	118
N10 -RU2 -N12 -C49 154.00 6.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	119
N11 -RU2 -N12 -C49 -117.00 6.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	120
N9 -RU2 -N12 -C49 62.00 6.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	189
RU1 -N6 -C24 -C25 -100.00 24.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	258
RU2 -N12 -C49 -C50 120.00 21.00 1.555 1.555 1.555	1.555
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	2
C25 H24 N6 Ru	
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	5
F6 P	
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	6
F6 P	

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
29 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
27 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

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 05/11/2012; check.def file version of 05/11/2012

