

# 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: kyo10

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Bond precision:    C-C = 0.0051 A                      Wavelength=0.71073

Cell:                      a=9.7749(10)              b=21.936(2)              c=13.4714(14)

                            alpha=90                      beta=90                      gamma=90

Temperature:              120 K

	Calculated	Reported
Volume	2888.6(5)	2888.6(5)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	?
Moiety formula	C23 H21 Cl N5 O4 Ru, F6 P	?
Sum formula	C23 H21 Cl F6 N5 O4 P Ru	C23 H21 Cl F6 N5 O4 P Ru
Mr	712.94	712.94
Dx,g cm-3	1.639	1.639
Z	4	4
Mu (mm-1)	0.768	0.768
F000	1424.0	1424.0
F000'	1420.75	
h,k,lmax	13,29,18	13,28,17
Nref	3749	3546
Tmin,Tmax	0.855,0.933	0.855,0.934
Tmin'	0.851	

Correction method= MULTI-SCAN

Data completeness= 0.946                      Theta(max)= 28.500

R(reflections)= 0.0442( 2914)              wR2(reflections)= 0.1345( 3546)

S = 1.113                      Npar= 205

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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.

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### Alert level B

PLAT029_ALERT_3_B _diffn_measured_fraction_theta_full	Low .....	0.946
PLAT230_ALERT_2_B Hirshfeld Test Diff for Cl1 -- O5 ..		14.0 su

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### ● Alert level C

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	Cl1	--	O6	..	7.0	su
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of						P1
PLAT431_ALERT_2_C	Short Inter HL..A Contact	F3	..	O5	.	2.87	Ang.
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of					91	A**3

### ● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained Atom Sites ....						2
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF						?
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.					7.13	
PLAT104_ALERT_1_G	The Reported Crystal System is Inconsistent with					Pnma	
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 ....						?
PLAT301_ALERT_3_G	Note: Main Residue Disorder .....					6	Perc.
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						6
	N1 -RU1 -O1 -CL1	180.00	0.02	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						15
	O1 -RU1 -N1 -C7	61.50	0.20	1.555	1.555	1.555	8.565
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						20
	O1 -RU1 -N1 -C7	-61.50	0.20	1.555	1.555	1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #						25
	O1 -RU1 -N1 -C1	180.00	0.01	1.555	1.555	1.555	1.555
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #						39
	O6 -CL1 -O5	8.565	1.555	8.565		43.50	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #						44
	O6 -CL1 -O5	1.555	1.555	1.555		43.50	Deg.
PLAT793_ALERT_4_G	The Model has Chirality at N1 (Verify) ....						R
PLAT793_ALERT_4_G	The Model has Chirality at C1 (Verify) ....						R
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints .....						12

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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
6 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 ALERT type 3 Indicator that the structure quality may be low  
9 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.

