

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) AG12_22_0m

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: AG12_22_0m

Bond precision: C-C = 0.0093 Å Wavelength=0.71073

Cell: a=10.5346(15) b=12.1661(16) c=14.845(2)
 alpha=104.711(8) beta=104.567(7) gamma=101.525(8)
Temperature: 296 K

	Calculated	Reported
Volume	1709.0(4)	1708.9(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C17 H15 Ru, F6 P	?
Sum formula	C17 H15 F6 P Ru	C34 H30 F12 P2 Ru2
Mr	465.33	930.66
Dx, g cm ⁻³	1.809	1.809
Z	4	2
Mu (mm ⁻¹)	1.068	1.068
F000	920.0	920.0
F000'	915.92	
h, k, lmax	12, 14, 17	12, 14, 17
Nref	6034	6029
Tmin, Tmax	0.880, 0.938	0.556, 0.747
Tmin'	0.726	

Correction method= # Reported T Limits: Tmin=0.556 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 24.998

R(reflections)= 0.0403(4012)	wR2(reflections)=
S = 1.004	0.1031(6029)
Npar= 525	

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

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.169

PLAT213_ALERT_2_C	Atom C2B'	has ADP max/min Ratio	3.3	oblate
PLAT234_ALERT_4_C	Large Hirshfeld Difference C1A	--C2A	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Ru2	--C2B'	0.18	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C14B	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Ru1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Ru2	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	P1	0.126	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	P2	0.108	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds		0.00931	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		6.914	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).		5	Note

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	20	Report
PLAT020_ALERT_3_G	The Value of Rint is Greater Than 0.12	0.169	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	2	Check
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0300	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0300	Report
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
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	28%	Note
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 2)	28%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	20	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	312	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3	Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	43%	Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities		Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	50.0	Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

18 **ALERT level G** = General information/check it is not something unexpected

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

8 ALERT type 2 Indicator that the structure model may be wrong or deficient

11 ALERT type 3 Indicator that the structure quality may be low

7 ALERT type 4 Improvement, methodology, query or suggestion

2 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* 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.

