

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: phw1202

Bond precision: C-C = 0.0059 Å

Wavelength=0.71070

Cell: a=10.5125(7) b=12.8761(8) c=13.0224(9)
 alpha=102.955(6) beta=110.920(6) gamma=107.384(6)
Temperature: 110 K

	Calculated	Reported
Volume	1459.1(2)	1459.07(16)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 H26.49 N6 Ru, 2(Cl)	C24 H26.49 N6 Ru, 2(Cl)
Sum formula	C24 H26.49 Cl2 N6 Ru	C24 H26.49 Cl2 N6 Ru
Mr	570.97	570.97
Dx,g cm ⁻³	1.300	1.300
Z	2	2
Mu (mm ⁻¹)	0.741	0.741
F000	581.0	581.0
F000'	579.18	
h,k,lmax	15,19,19	15,18,18
Nref	10250	9142
Tmin,Tmax	0.888,0.949	0.896,0.960
Tmin'	0.833	

Correction method= ANALYTICAL

Data completeness= 0.892

Theta(max)= 32.140

R(reflections)= 0.0491(7712)

wR2(reflections)= 0.1330(9142)

S = 1.033

Npar= 312

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 A

PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of . 347 Ang³

Alert level C

PLAT414_ALERT_2_C Short Intra D-H..H-X H4B .. H3B .. 1.96 Ang.

● Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	? Do !
PLAT007_ALERT_5_G	Note: Number of Unrefined Donor-H Atoms	1
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	4 Units
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal	0.00600 Deg.
PLAT301_ALERT_3_G	Note: Main Residue Disorder	6 %
PLAT302_ALERT_4_G	Note: Anion/Solvent Disorder	50 %
PLAT793_ALERT_4_G	The Model has Chirality at N2 (Verify)	R
PLAT793_ALERT_4_G	The Model has Chirality at C1 (Verify)	R
PLAT793_ALERT_4_G	The Model has Chirality at C3 (Verify)	S
PLAT793_ALERT_4_G	The Model has Chirality at C5 (Verify)	S

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
5 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*, 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.

