

## checkCIF (basic structural check) running

### checkCIF/PLATON (basic structural check)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found.  
Please wait while processing ....

[CIF dictionary](#)  
[Interpreting this report](#)

## Datablock: cpx21b

Bond precision:	C-C = 0.0075 A	Wavelength=0.71073
Cell:	a=8.3490(5)      b=29.5901(12)      c=16.8571(7)	
	alpha=90      beta=97.391(4)      gamma=90	
Temperature:	296 K	
	Calculated	Reported
Volume	4129.9(3)	4129.9(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C34 H39 Cl2 N4 O Rh2, F6 P, C H2 Cl2	C34 H39 Cl2 N4 O Rh2, F6 P, C H2 Cl2
Sum formula	C35 H41 Cl4 F6 N4 O P Rh2	C35 H41 Cl4 F6 N4 O P Rh2
Mr	1026.31	1026.31
Dx,g cm-3	1.651	1.651
Z	4	4
Mu (mm-1)	1.157	1.157
F000	2056.0	2056.0
F000'	2050.64	
h,k,lmax	11,40,22	11,38,21
Nref	10743	9453
Tmin,Tmax	0.933,0.944	0.903,0.944
Tmin'	0.901	
Correction method=	# Reported T Limits: Tmin=0.903 Tmax=0.944 AbsCorr =	
	MULTI-SCAN	
Data completeness=	0.880	Theta(max)= 28.770
R(reflections)=	0.0557( 5965)	wR2(reflections)= 0.0989( 9453)
S =	1.034	Npar= 558

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

<a href="#">PLAT213_ALERT_2_C</a>	Atom C18	has ADP max/min Ratio .....	3.1	prolat
<a href="#">PLAT220_ALERT_2_C</a>	Non-Solvent Resd 1	C Ueq(max)/Ueq(min) Range	4.3	Ratio
<a href="#">PLAT220_ALERT_2_C</a>	Non-Solvent Resd 1	N Ueq(max)/Ueq(min) Range	3.5	Ratio
<a href="#">PLAT222_ALERT_3_C</a>	Non-Solvent Resd 1	H Uiso(max)/Uiso(min) Range	5.0	Ratio

### ● Alert level G

<a href="#">PLAT002_ALERT_2_G</a>	Number of Distance or Angle Restraints on AtSite	19	Note
<a href="#">PLAT066_ALERT_1_G</a>	Predicted and Reported Tmin&Tmax Range Identical	?	Check
<a href="#">PLAT171_ALERT_4_G</a>	The CIF-Embedded .res File Contains EADP Records	2	Report
<a href="#">PLAT175_ALERT_4_G</a>	The CIF-Embedded .res File Contains SAME Records	2	Report
<a href="#">PLAT244_ALERT_4_G</a>	Low 'Solvent' Ueq as Compared to Neighbors of	P1	Check
<a href="#">PLAT300_ALERT_4_G</a>	Atom Site Occupancy of *H6A is Constrained at	0.5	Check

#### And 5 other PLAT300 Alerts

More ...

<a href="#">PLAT302_ALERT_4_G</a>	Anion/Solvent Disorder .....	Percentage =	90	Note
<a href="#">PLAT304_ALERT_4_G</a>	Non-Integer Number of Atoms ( 4.22) in Resd. #		3	Check
<a href="#">PLAT304_ALERT_4_G</a>	Non-Integer Number of Atoms ( 0.78) in Resd. #		4	Check

PLAT721_ALERT_1_G Bond Calc	0.95000, Rep	0.97000 Dev...	0.02 Ang.
C35B -H35C	1.555 1.555 .....	Bond # 117	Check
PLAT721_ALERT_1_G Bond Calc	1.01000, Rep	0.97000 Dev...	0.04 Ang.
C35B -H35D	1.555 1.555 .....	Bond # 118	Check
PLAT722_ALERT_1_G Angle Calc	112.00, Rep	110.50 Dev...	1.50 Degree
CL4B -C35B -H35C	1.555 1.555 1.555	# 315	
PLAT722_ALERT_1_G Angle Calc	112.00, Rep	110.50 Dev...	1.50 Degree
CL3B -C35B -H35C	1.555 1.555 1.555	# 316	
PLAT722_ALERT_1_G Angle Calc	109.00, Rep	110.50 Dev...	1.50 Degree
CL4B -C35B -H35D	1.555 1.555 1.555	# 317	
PLAT722_ALERT_1_G Angle Calc	109.00, Rep	110.50 Dev...	1.50 Degree
CL3B -C35B -H35D	1.555 1.555 1.555	# 318	
PLAT722_ALERT_1_G Angle Calc	107.00, Rep	108.70 Dev...	1.70 Degree
H35C -C35B -H35D	1.555 1.555 1.555	# 319	
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #			262 Check
F6B -P1 -F6	1.555 1.555 1.555	16.80 Deg.	
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #			266 Check
F4 -P1 -F3B	1.555 1.555 1.555	37.80 Deg.	
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #			276 Check
F2B -P1 -F3	1.555 1.555 1.555	34.60 Deg.	
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #			291 Check
F5 -P1 -F5B	1.555 1.555 1.555	12.40 Deg.	
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #			295 Check
F1B -P1 -F2	1.555 1.555 1.555	42.90 Deg.	
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....			24 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL			2014 Note
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ			2 Units

0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 0 **ALERT level B** = A potentially serious problem, consider carefully  
 4 **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

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 4 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  
 18 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

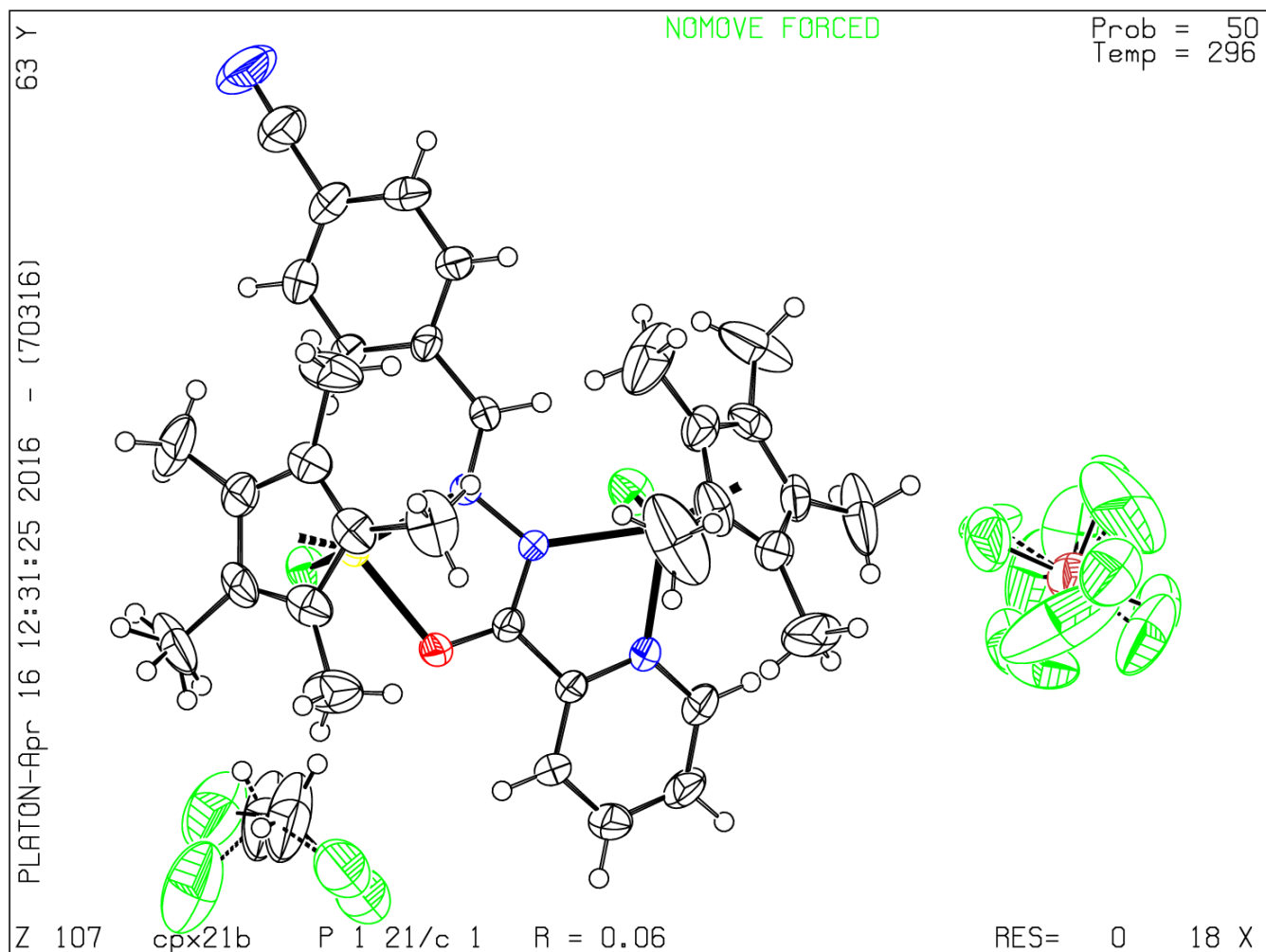
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* 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.

PLATON version of 30/03/2016; check.def file version of 30/03/2016

## Datablock cpx21b - ellipsoid plot



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