

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait ...

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) 2pcpx46

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.
Please wait while processing

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

[Structure factor report](#)

Datablock: 2pcpx46

Bond precision:	C-C = 0.0093 Å	Wavelength=0.71073
Cell:	a=7.5644(4) b=22.2101(9) c=21.1554(11)	
	alpha=90 beta=92.497(5) gamma=90	
Temperature:	293 K	
	Calculated	Reported
Volume	3550.9(3)	3550.9(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C33 H29 Cl2 N2 Rh, C H Cl3	0.8(C33 H29 Cl2 N2 Rh), 0.8(C H Cl3)
Sum formula	C34 H30 Cl5 N2 Rh	C27.20 H24 Cl4 N1.60 Rh0.80
Mr	746.76	597.41
Dx, g cm ⁻³	1.397	1.397
Z	4	5
Mu (mm ⁻¹)	0.882	0.882
F000	1512.0	1512.0
F000'	1510.85	
h,k,lmax	9,27,26	9,27,26
Nref	7268	7255
Tmin,Tmax	0.831,0.861	0.736,1.000
Tmin'	0.831	
Correction method= # Reported T Limits: Tmin=0.736 Tmax=1.000 AbsCorr = MULTI-SCAN		
Data completeness=	0.998	Theta(max)= 26.371
R(reflections)=	0.0634(3718)	wR2(reflections)= 0.1400(7255)
S =	0.978	Npar= 383

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 B

[PLAT910_ALERT_3_B](#) Missing # of FCF Reflection(s) Below Theta(Min) 11 Note

Alert level C

[PLAT213_ALERT_2_C](#) Atom C9 has ADP max/min Ratio 3.3 prolat
[PLAT220_ALERT_2_C](#) Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.1 Ratio
[PLAT222_ALERT_3_C](#) Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 4.5 Ratio

PLAT234_ALERT_4_C Large Hirshfeld Difference C0AA -- C10 .. 0.19 Ang.
 PLAT234_ALERT_4_C Large Hirshfeld Difference C4 -- C8 .. 0.17 Ang.
 PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Rh1 Check
 PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C3AA Check
 PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.00929 Ang.
 PLAT906_ALERT_3_C Large K value in the Analysis of Variance 5.872 Check
 PLAT906_ALERT_3_C Large K value in the Analysis of Variance 2.405 Check
 PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 2 Report

●Alert level G

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
 PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.80 Check
 PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
 PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
 PLAT605_ALERT_4_G Largest Solvent Accessible VOID in Structure ... 156 A**3
 PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 6 Note
 PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
 C H Cl3
 PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed ! Info

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

- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 3 ALERT type 2 Indicator that the structure model may be wrong or deficient
 6 ALERT type 3 Indicator that the structure quality may be low
 7 ALERT type 4 Improvement, methodology, query or suggestion
 0 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

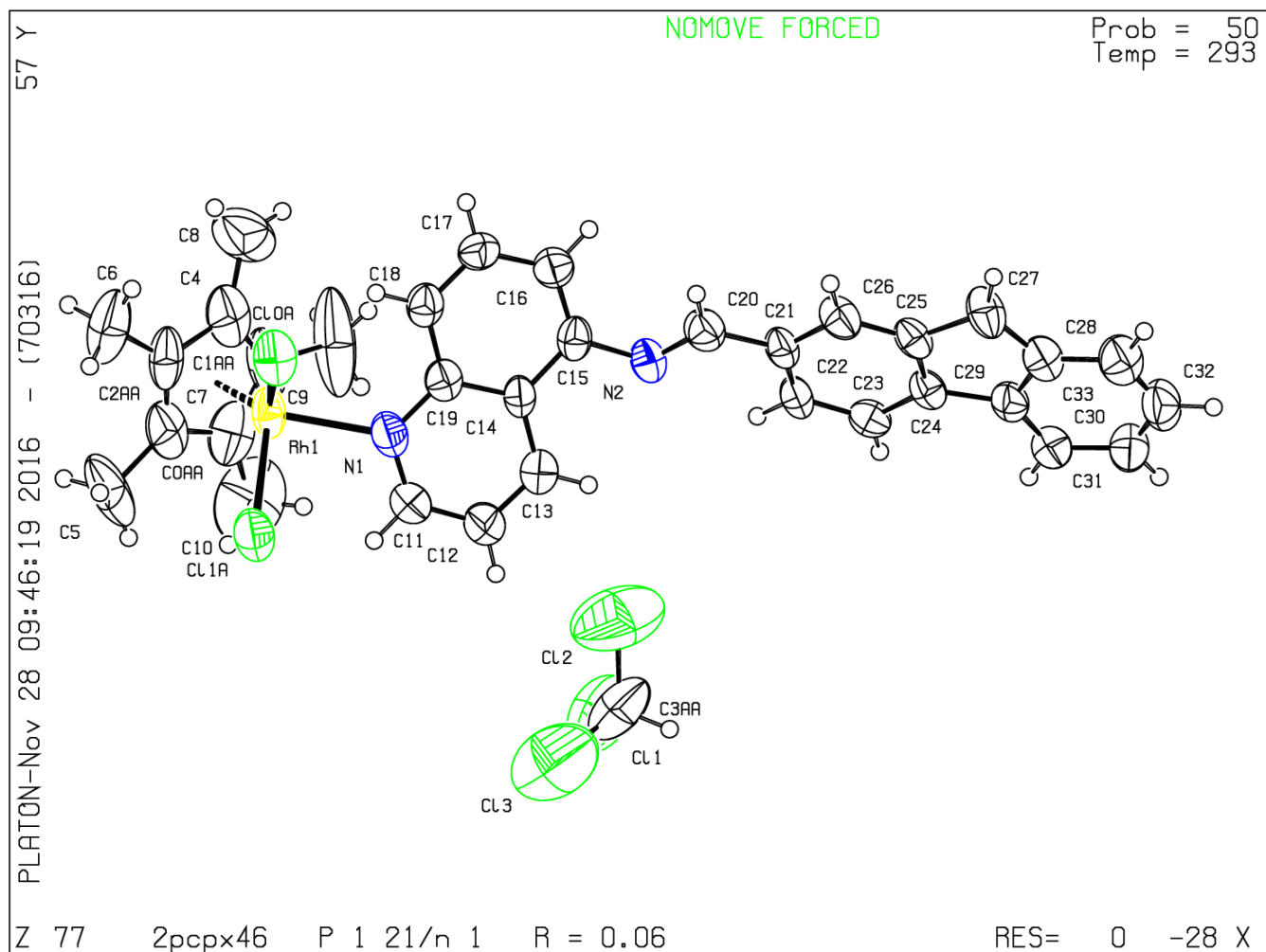
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 11/08/2016; check.def file version of 04/08/2016

Datablock 2pcpx46 - ellipsoid plot



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