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. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: kmrnr-28

Bond precision: C-C = 0.0151 A Wavelength=0.71073

Cell: a=16.9838(9) b=7.9705(6) c=38.6554(18)
alpha=90 beta=90 gamma=90

Temperature: 291 K

	Calculated	Reported
Volume	5232.8(5)	5232.7(5)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C30 H29 Cl N3 O Rh	C30 H29 Cl N3 O Rh
Sum formula	C30 H29 Cl N3 O Rh	C30 H29 Cl N3 O Rh
Mr	585.92	585.92
Dx,g cm-3	1.487	1.487
Z	8	8
Mu (mm-1)	0.783	0.783
F000	2400.0	2400.0
F000'	2392.93	
h,k,lmax	22,10,52	21,10,48
Nref	13551[6875]	9163
Tmin,Tmax	0.885,0.969	0.832,1.000
Tmin'	0.687	

Correction method= # Reported T Limits: Tmin=0.832 Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 1.33/0.68 Theta(max)= 28.719

R(reflections)= 0.0628(7525) wR2(reflections)= 0.1304(9163)

S = 1.104 Npar= 603

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

PLAT987_ALERT_1_B The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

Alert level C

CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.470
From the CIF: _refine_ls_abs_structure_Flack_su 0.030
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.4 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range 3.5 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C11 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Rh2 Check
PLAT334_ALERT_2_C Small Average Benzene C-C Dist. C12 -C17 1.37 Ang.
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01511 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact H9 .. H43 .. 2.12 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact H13 .. H50' .. 2.08 Ang.
PLAT732_ALERT_1_C Angle Calc 37.93(19), Rep 37.90(7) ..... 2.71 s.u.-R
C52 -RH2 -C51 1.555 1.555 1.555 # 174

PLAT732_ALERT_1_C Angle Calc 38.99(19), Rep 39.00(7) ..... 2.71 s.u.-R
C53 -RH2 -C52 1.555 1.555 1.555 # 177
PLAT732_ALERT_1_C Angle Calc 37.73(18), Rep 37.73(8) ..... 2.25 s.u.-R
C53 -RH2 -C54 1.555 1.555 1.555 # 178
PLAT732_ALERT_1_C Angle Calc 36.98(17), Rep 36.99(7) ..... 2.43 s.u.-R
C55 -RH2 -C51 1.555 1.555 1.555 # 184
PLAT732_ALERT_1_C Angle Calc 38.63(17), Rep 38.63(7) ..... 2.43 s.u.-R
C55 -RH2 -C54 1.555 1.555 1.555 # 186
PLAT732_ALERT_1_C Angle Calc 70.3(3), Rep 70.35(13) ..... 2.31 s.u.-R
C52 -C51 -RH2 1.555 1.555 1.555 # 302
PLAT732_ALERT_1_C Angle Calc 70.1(3), Rep 70.07(13) ..... 2.31 s.u.-R
C55 -C51 -RH2 1.555 1.555 1.555 # 304
PLAT732_ALERT_1_C Angle Calc 126.6(4), Rep 126.59(15) ..... 2.67 s.u.-R
C56 -C51 -RH2 1.555 1.555 1.555 # 307
PLAT732_ALERT_1_C Angle Calc 71.8(3), Rep 71.75(14) ..... 2.14 s.u.-R
C51 -C52 -RH2 1.555 1.555 1.555 # 308
PLAT732_ALERT_1_C Angle Calc 127.1(3), Rep 127.09(12) ..... 2.50 s.u.-R
C57 -C52 -RH2 1.555 1.555 1.555 # 313
PLAT732_ALERT_1_C Angle Calc 124.3(4), Rep 124.26(14) ..... 2.86 s.u.-R
C58 -C53 -RH2 1.555 1.555 1.555 # 319
PLAT732_ALERT_1_C Angle Calc 70.0(3), Rep 69.97(12) ..... 2.50 s.u.-R
C53 -C54 -RH2 1.555 1.555 1.555 # 320
PLAT732_ALERT_1_C Angle Calc 125.4(3), Rep 125.45(13) ..... 2.31 s.u.-R
C59 -C54 -RH2 1.555 1.555 1.555 # 325
PLAT732_ALERT_1_C Angle Calc 73.0(3), Rep 72.94(14) ..... 2.14 s.u.-R
C51 -C55 -RH2 1.555 1.555 1.555 # 326
PLAT732_ALERT_1_C Angle Calc 128.2(3), Rep 128.23(12) ..... 2.50 s.u.-R
C60 -C55 -RH2 1.555 1.555 1.555 # 331

Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 7.73 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 13 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 18 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 1604 Note
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ 4 Units

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
25 **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

17 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
3 ALERT type 3 Indicator that the structure quality may be low
5 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 kmrnr-28 - ellipsoid plot

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