checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C3

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: C3

Bond precision: C-C = 0.0041 A Wavelength=0.71073

Cell: a=14.4642(10) b=17.4776(11) c=24.9801(17)
alpha=90 beta=97.812(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	6256.4(7)	6256.3(7)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C28 H30 Cl N2 O4 Rh, C28 H29 Cl N2 O4 Rh, 2(Cl), 3(H2 O) [+ sol	C28 H30 Cl N2 O4 Rh, C28 H29 Cl N2 O4 Rh, 3(H2 O), 2(Cl)
Sum formula	C56 H65 Cl4 N4 O11 Rh2 [+ solvent]	C56 H65 Cl4 N4 O11 Rh2
Mr	1317.74	1317.74
Dx,g cm-3	1.399	1.399
Z	4	4
Mu (mm-1)	0.755	0.755
F000	2700.0	2700.0
F000’	2694.44	
h,k,lmax	19,23,33	19,23,33
Nref	15631	15594
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 0.998 Theta(max)= 28.340

R(reflections)= 0.0454(13073) wR2(reflections)= 0.1205(15594)

S = 1.035 Npar= 724

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

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PLAT260_ALERT_2_B Large Average Ueq of Residue Including       Cl2      0.615 Check
PLAT350_ALERT_3_B Short  C-H (X0.96,N1.08A)  C023     - H02H     .       0.71 Ang.
PLAT420_ALERT_2_B D-H Without Acceptor       O2AA     --H2AB     .     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O2AA     --H2AC     .     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O1A      --H1AB     .     Please Check
PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ...          2 Check
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....          2 Check
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Alert level C

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PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...     Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...     Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...     Please Check
PLAT213_ALERT_2_C Atom O00P            has ADP max/min Ratio .....        4.0 prolat
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl1      0.272 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O1A      0.114 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O2AA      0.178 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for ..........       C023 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          2 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          2 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.05A   From C023           0.71 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.62A   From O2AA          -0.98 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.89A   From O2AA          -0.95 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.57A   From O2AA          -0.94 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  1.02A   From O1A           -0.43 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2AB            -0.59 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2AC            -0.31 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
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Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          8 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      21.55 Why ?
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C023 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  Cl1      ..O00P     .       2.87 Ang.
                                              1-x,1-y,1-z  =      3_666 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  Cl1      ..O008     .       2.96 Ang.
                                              1-x,1-y,1-z  =      3_666 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl2      ..Cl2              2.66 Ang.
                                               1-x,-y,1-z  =      3_656 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure       268 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       135 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed         ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        37 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   7 ALERT level B = A potentially serious problem, consider carefully
  19 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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 22 ALERT type 2 Indicator that the structure model may be wrong or deficient
  5 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
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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 03/05/2019; check.def file version of 29/04/2019

Datablock C3 - ellipsoid plot