

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu\_20240531b\_a

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: cu\_20240531b\_a

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Bond precision:      C-C = 0.0194 Å

Wavelength=1.54178

Cell:                      a=15.1059(5)                      b=22.4303(9)                      c=37.6847(13)  
                              alpha=75.117(2)                      beta=87.804(2)                      gamma=71.666(2)  
Temperature:              153 K

|                        | Calculated                        | Reported                                  |
|------------------------|-----------------------------------|-------------------------------------------|
| Volume                 | 11701.4(8)                        | 11701.4(7)                                |
| Space group            | P -1                              | P -1                                      |
| Hall group             | -P 1                              | -P 1                                      |
| Moiety formula         | C104 H98 N6 O8 Rh4 [+<br>solvent] | 2(C104 H98 N6 O8 Rh4),<br>9[CF3SO3]       |
| Sum formula            | C104 H98 N6 O8 Rh4 [+<br>solvent] | C108.50 H98 F13.50 N6<br>O21.50 Rh4 S4.50 |
| Mr                     | 1971.53                           | 2642.33                                   |
| Dx, g cm <sup>-3</sup> | 1.119                             | 1.500                                     |
| Z                      | 4                                 | 4                                         |
| Mu (mm <sup>-1</sup> ) | 4.857                             | 6.005                                     |
| F000                   | 4032.0                            | 5346.0                                    |
| F000'                  | 4043.28                           |                                           |
| h, k, lmax             | 15, 22, 37                        | 15, 22, 37                                |
| Nref                   | 24569                             | 24438                                     |
| Tmin, Tmax             | 0.467, 0.406                      |                                           |
| Tmin'                  | 0.353                             |                                           |

Correction method= Not given

Data completeness= 0.995

Theta(max)= 50.483

R(reflections)= 0.0922( 15490)

wR2(reflections)=  
0.2036( 24438)

S = 1.031

Npar= 2042

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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.

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### Alert level A

THETM01\_ALERT\_3\_A The value of sine(theta\_max)/wavelength is less than 0.550

Calculated sin(theta\_max)/wavelength = 0.5004

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### Alert level C

PLAT052\_ALERT\_1\_C Info on Absorption Correction Method Not Given Please Do !

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.7 Ratio

PLAT220\_ALERT\_2\_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 4.4 Ratio

PLAT222\_ALERT\_3\_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.6 Ratio

PLAT222\_ALERT\_3\_C NonSolvent Resd 2 H Uiso(max)/Uiso(min) Range 5.2 Ratio

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference Rh7 --O7 . 0.16 Ang.

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of O11 Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of O15 Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C51 Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C91 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Rh9 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Rh7 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of N2 Check

PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including Rh5 0.128 Check

PLAT334\_ALERT\_2\_C Small <C-C> Benzene Dist. C15 -C137 . 1.37 Ang.

PLAT342\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.01942 Ang.

PLAT369\_ALERT\_2\_C Long C(sp2)-C(sp2) Bond C53 - C171 . 1.56 Ang.

PLAT369\_ALERT\_2\_C Long C(sp2)-C(sp2) Bond C27 - C190 . 1.55 Ang.

PLAT410\_ALERT\_2\_C Short Intra H...H Contact H14 ..H96 . 1.95 Ang.

PLAT410\_ALERT\_2\_C Short Intra H...H Contact H18 ..H50 . 1.96 Ang.

PLAT410\_ALERT\_2\_C Short Intra H...H Contact H85 ..H156 . 1.92 Ang.

PLAT410\_ALERT\_2\_C Short Intra H...H Contact H2 ..H17 . 1.97 Ang.

PLAT410\_ALERT\_2\_C Short Intra H...H Contact H146 ..H202 . 1.98 Ang.

PLAT410\_ALERT\_2\_C Short Intra H...H Contact H155 ..H188 . 1.96 Ang.

PLAT410\_ALERT\_2\_C Short Intra H...H Contact H186 ..H194 . 1.94 Ang.

PLAT413\_ALERT\_2\_C Short Inter XH3 .. XHn H23A ..H37B . 2.05 Ang.

2-x,1-y,1-z = 2\_766 Check

PLAT420\_ALERT\_2\_C D-H Bond Without Acceptor N3 --H3 . Please Check

PLAT420\_ALERT\_2\_C D-H Bond Without Acceptor N5 --H5 . Please Check

PLAT420\_ALERT\_2\_C D-H Bond Without Acceptor N7 --H7 . Please Check

PLAT420\_ALERT\_2\_C D-H Bond Without Acceptor N10 --H10D . Please Check

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.500 126 Report

1 0 0, -1 1 0, 1 1 0, 15 9 0, 14 14 0, 5-17 1,

-1 -5 1, -2 -3 1, -1 -2 1, 0 -1 1, 1 0 1, -2 1 1,

2 1 1, 0 2 1, -2 4 1, 1 5 1, -10 11 1, -15 -8 2,

-1 -2 2, 0 -2 2, -2 -1 2, -1 -1 2, -1 1 2, 0 1 2,

1 3 2, 1 4 2, -2-19 3, -15 -7 3, -15 -6 3, -1 -1 3,

-1 0 3, 0 0 3, 1 0 3, -3 1 3, 0 2 3, 6 22 3,

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-2 -3 4, 0 1 4, 1 1 4, 1 2 4, 10-10 5, -2 -1 5,
-1 -1 5, 1 0 5, -2 3 5, 15 6 5, 15 9 5, 1 0 6,
0 1 6, 1 1 6, -2 2 6, -1 5 6, 15 8 6, -9-19 7,
1 0 7, -10-18 8, -14-11 8, 0 -1 8, 1 4 8, 0 8 8,
12 -5 9, 4 3 9, -2 4 9, -7-19 10, 6-14 10, 13 -2 10,
-1 2 11, -14 -2 12, 14 3 12, 6-13 13, -13-11 13, -8 14 13,
-2 20 14, -6 16 17, 5-12 18, 13 12 18, 12 16 19, -1 20 19,
13 11 20, 11 17 21, 6 21 21, -4 17 22, 10 18 22, -10 7 23,
-7 13 23, -9-10 24, 11 2 24, -6 14 24, -9 -9 25, 6 -7 25,
10 7 25, -7 12 25, -4 16 25, 3 20 25, -6-11 26, -5 14 27,
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 3 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.92Ang From O11 1.66 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H10A . -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H10B . -0.34 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H51B . -0.39 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H51C . -0.53 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H173 . -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H204 . -0.39 eA-3

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## Alert level G

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FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
    _chemical_formula_sum and _chemical_formula_moiety. This is
    usually due to the moiety formula being in the wrong format.
    Atom count from _chemical_formula_sum: C108.5 H98 F13.5 N6 O21.5 Rh4
    Atom count from _chemical_formula_moiety: C217 H196 F27 N12 O43 Rh8 S9
FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
    _chemical_formula_sum and the formula from the _atom_site* data.
    Atom count from _chemical_formula_sum: C108.5 H98 F13.5 N6 O21.5 Rh4 S4
    Atom count from the _atom_site data: C104 H98 N6 O8 Rh4
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
    symmetry error - see SYMMG tests
    From the CIF: _cell_formula_units_Z 4
    From the CIF: _chemical_formula_sum C108.50 H98 F13.50 N6 O21.50 Rh4 S
    TEST: Compare cell contents of formula and atom_site data

atom      Z*formula  cif sites diff
C          434.00    416.00  18.00
H          392.00    392.00   0.00
F           54.00     0.00  54.00
N           24.00    24.00   0.00
O           86.00    32.00  54.00
Rh          16.00    16.00   0.00
S           18.00     0.00  18.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 35 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms 245 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 4 Report
      H3      H7      H5      H10D
PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
      Calc: C104 H98 N6 O8 Rh4
      Rep.: C108.50 H98 F13.50 N6 O21.50 Rh4 S4.50
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
      Calc: C104 H98 N6 O8 Rh4
      Rep.: 2(C104 H98 N6 O8 Rh4), 9[CF3SO3]
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 19.12 %
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 150.00 Why ?

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|                   |                                                     |               |
|-------------------|-----------------------------------------------------|---------------|
| PLAT154_ALERT_1_G | The s.u.'s on the Cell Angles are Equal ..(Note)    | 0.002 Degree  |
| PLAT172_ALERT_4_G | The CIF-Embedded .res File Contains DFIX Records    | 12 Report     |
| PLAT173_ALERT_4_G | The CIF-Embedded .res File Contains DANG Records    | 12 Report     |
| PLAT174_ALERT_4_G | The CIF-Embedded .res File Contains FLAT Records    | 3 Report      |
| PLAT176_ALERT_4_G | The CIF-Embedded .res File Contains SADI Records    | 12 Report     |
| PLAT177_ALERT_4_G | The CIF-Embedded .res File Contains DELU Records    | 1 Report      |
| PLAT178_ALERT_4_G | The CIF-Embedded .res File Contains SIMU Records    | 4 Report      |
| PLAT186_ALERT_4_G | The CIF-Embedded .res File Contains ISOR Records    | 1 Report      |
| PLAT187_ALERT_4_G | The CIF-Embedded .res File Contains RIGU Records    | 3 Report      |
| PLAT188_ALERT_3_G | A Non-default SIMU Restraint Value has been used    | 0.0100 Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used    | 0.0400 Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used    | 0.0400 Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used    | 0.0400 Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used    | 0.0400 Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used    | 0.0400 Report |
| PLAT191_ALERT_3_G | A Non-default SADI Restraint Value has been used    | 0.0400 Report |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Rh2 --O11 .               | 8.0 s.u.      |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Rh2 --N11 .               | 10.5 s.u.     |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Rh2 --C25 .               | 5.5 s.u.      |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Rh2 --C51 .               | 8.4 s.u.      |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Rh2 --C101 .              | 9.0 s.u.      |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Rh2 --C201 .              | 8.5 s.u.      |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Rh3 --O11 .               | 5.5 s.u.      |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Rh3 --O15 .               | 10.5 s.u.     |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Rh3 --N11 .               | 10.0 s.u.     |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Rh3 --C25 .               | 10.2 s.u.     |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Rh3 --C99 .               | 11.0 s.u.     |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Rh3 --C101 .              | 8.2 s.u.      |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Rh3 --C199 .              | 6.2 s.u.      |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Rh3 --C201 .              | 7.2 s.u.      |
| PLAT301_ALERT_3_G | Main Residue Disorder .....(Resd 1)                 | 1% Note       |
| PLAT333_ALERT_2_G | Large Aver C6-Ring C-C Dist C19 -C159 .             | 1.43 Ang.     |
| PLAT335_ALERT_2_G | Check Large C6 Ring C-C Range C36 -C182             | 0.15 Ang.     |
| PLAT335_ALERT_2_G | Check Large C6 Ring C-C Range C19 -C159             | 0.19 Ang.     |
| PLAT335_ALERT_2_G | Check Large C6 Ring C-C Range C69 -C141             | 0.16 Ang.     |
| PLAT380_ALERT_4_G | Incorrectly? Oriented X(sp2)-Methyl Moiety .....    | C23 Check     |
| PLAT380_ALERT_4_G | Incorrectly? Oriented X(sp2)-Methyl Moiety .....    | C197 Check    |
| PLAT380_ALERT_4_G | Incorrectly? Oriented X(sp2)-Methyl Moiety .....    | C93 Check     |
| PLAT606_ALERT_4_G | Solvent Accessible VOID(S) in Structure .....       | ! Info        |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints .....            | 3273 Note     |
| PLAT868_ALERT_4_G | ALERTS Due to the Use of _smtbx_masks Suppressed    | ! Info        |
| PLAT883_ALERT_1_G | No Info/Value for _atom_sites_solution_primary .    | Please Do !   |
| PLAT909_ALERT_3_G | Percentage of I>2sig(I) Data at Theta(Max) Still    | 34% Note      |
| PLAT910_ALERT_3_G | Missing # of FCF Reflection(s) Below Theta(Min).    | 2 Note        |
|                   | 0 1 0, 0 0 1,                                       |               |
| PLAT913_ALERT_3_G | Missing # of Very Strong Reflections in FCF ....    | 1 Note        |
|                   | 0 -2 2,                                             |               |
| PLAT933_ALERT_2_G | Number of HKL-OMIT Records in Embedded .res File    | 47 Note       |
|                   | -3 1 3, -2 -3 1, -2 -3 4, -2 -1 2, -2 -1 5, -2 2 6, |               |
|                   | -2 3 5, -2 4 1, -2 4 9, -1 -5 1, -1 -2 1, -1 -2 2,  |               |
|                   | -1 -1 2, -1 -1 3, -1 -1 5, -1 0 3, -1 1 0, -1 1 2,  |               |
|                   | -1 2 11, -1 5 6, 0 -2 2, 0 -1 1, 0 -1 8, 0 0 3,     |               |
|                   | 0 1 0, 0 1 2, 0 1 4, 0 1 6, 0 2 1, 0 2 3,           |               |
|                   | 0 8 8, 1 0 0, 1 0 1, 1 0 3, 1 0 5, 1 0 6,           |               |
|                   | 1 0 7, 1 1 0, 1 1 4, 1 1 6, 1 2 4, 1 3 2,           |               |
|                   | 1 4 2, 1 4 8, 1 5 1, 2 1 1, 4 3 9,                  |               |
| PLAT969_ALERT_5_G | The 'Henn et al.' R-Factor-gap value .....          | 4.238 Note    |

Predicted wR2: Based on SigI\*\*2 4.81 or SHELX Weight 19.74  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 3 Info

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

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
56 ALERT type 2 Indicator that the structure model may be wrong or deficient  
18 ALERT type 3 Indicator that the structure quality may be low  
14 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

