checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mb_c_c_2_sq

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: mb_c_c_2_sq

Bond precision: C-C = 0.0109 A   Wavelength=1.54184

Cell: a=20.5437(4)   b=10.4027(4)   c=30.6083(9)
               alpha=90   beta=106.710(3)   gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	6265.1(3)	6265.1(3)
Space group	I 2	I 2
Hall group	I 2y	I 2y
Moiety formula	C48 H52 N4 O8 Rh, B F4 [+ solvent]	C48 H52 N4 O8 Rh +, B F4 −
Sum formula	C48 H52 B F4 N4 O8 Rh [+ solvent]	C48 H52 B F4 N4 O8 Rh
Mr	1002.66	1002.65
Dx,g cm−3	1.063	1.063
Z	4	4
Mu (mm−1)	2.669	2.669
F000	2072.0	2072.0
F000'	2078.90	
h,k,lmax	26,13,39	26,13,39
Nref	13657[7215]	10695
Tmin,Tmax	0.553,0.670	0.788,1.000
Tmin'	0.489	

Correction method= # Reported T Limits: Tmin=0.788 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.48/0.78   Theta(max)= 79.746

R(reflections)= 0.0344(9568)

wR2(reflections)= 0.1024(10695)

S = 1.120   Npar= 606

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**

PLAT260_ALERT_2_B Large Average Ueq of Residue Including   F1_3   0.339 Check
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..   6 Check
            19 -7 0, 20 6 0, -19 -7 2, -19 -7 4, -19 7 4, -17 -7 8,

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🟡 **Alert level C**

PLAT220_ALERT_2_C NonSolvent   Resd 1 C   Ueq(max)/Ueq(min) Range   3.1 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for   O2CA_1   --Cm_1   .   5.8 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for   C1C_2   --C4C_2_b .   7.0 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for   C4C_2   --C1C_2_b .   7.0 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference O1CA_1   --CcA_1   .   0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C3B1_1   --Cc1_1   .   0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O2CA_2   --Cm_2   .   0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference CaA_2   --CcA_2   .   0.16 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C5B1_1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C3C_1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C5B1_2 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   CcA_1 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   CcA_2 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd   1)   2.3 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   Rh_1   0.115 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.01086 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn   HmB_1   ..HbAA_2   .   2.11 Ang.
                                      -1+x,y,z   =   1_455 Check
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4   Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   51 Report
            0 6 0, 18 8 0,   3 2 1,   4 2 2, -11 4 3, -13 0 5,
          -11 0 5, -12 0 6, -10 0 6, 22 0 6, -13 0 7, -11 0 7,
          -12 0 8, -13 0 9, -11 0 9, 21 0 9, -15 9 10, -12 0 10,
           20 0 10, -13 0 11, -11 0 11, 17 0 11, 19 0 11, -12 0 12,
           16 0 12, 18 0 12, 17 0 13, 19 0 13, -12 0 14, 16 0 14,
           18 0 14, 15 0 15, 17 0 15, -12 0 16, 16 0 16, 18 0 16,
          -13 0 17, 13 0 17, 15 0 17, 17 0 17, 16 0 18, 13 0 19,
           15 0 19, -12 0 20, 12 0 20, 14 0 20, 15 0 21, 12 0 22,
           14 0 22, 13 0 23, -15 0 31,
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage   58 %

⚪ **Alert level G**

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   4 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)   293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K)   293 Check
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of   B1_3 Check
PLAT398_ALERT_2_G Deviating C-O-C   Angle From 120 for O1O_1   .   105.4 Degree

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PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O1O_2    .       105.5 Degree
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT791_ALERT_4_G Model has Chirality at C4O_1        (Sohncke SpGr)        R Verify
PLAT791_ALERT_4_G Model has Chirality at CaA_1        (Sohncke SpGr)        S Verify
PLAT791_ALERT_4_G Model has Chirality at C4O_2        (Sohncke SpGr)        R Verify
PLAT791_ALERT_4_G Model has Chirality at CaA_2        (Sohncke SpGr)        S Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         3 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL    2019/3 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         2 Note
                -1  0  1,   0  0  2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       202 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       4.0 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     2.870 Note
              Predicted wR2: Based on SigI**2  3.57 or SHELX Weight  9.20
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        1 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
  20 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  20 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  17 ALERT type 2 Indicator that the structure model may be wrong or deficient
   7 ALERT type 3 Indicator that the structure quality may be low
  15 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 13/05/2024; check.def file version of 15/07/2024

NOMOVE FORCED

Prob = 50
Temp = 293

23 Y

PLATON-Jul 24 13:42:48 2024 - (130524)

Z 178   mb_c_c_2_sq   I 2   R = 0.03   RES= 0 -89 X