

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) br1425, br1511, br1517b

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: br1425

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Bond precision:    C-C = 0.0094 Å

Wavelength=0.71073

Cell:                a=12.9211(11)                b=13.1846(13)                c=16.1976(13)  
                      alpha=102.947(8)            beta=103.219(7)            gamma=91.302(7)  
Temperature:    100 K

|                | Calculated       | Reported         |
|----------------|------------------|------------------|
| Volume         | 2610.0(4)        | 2610.0(4)        |
| Space group    | P -1             | P -1             |
| Hall group     | -P 1             | -P 1             |
| Moiety formula | C61 H44 N4 P2 Ru | C61 H44 N4 P2 Ru |
| Sum formula    | C61 H44 N4 P2 Ru | C61 H44 N4 P2 Ru |
| Mr             | 996.01           | 996.01           |
| Dx,g cm-3      | 1.267            | 1.267            |
| Z              | 2                | 2                |
| Mu (mm-1)      | 0.404            | 0.404            |
| F000           | 1024.0           | 1024.0           |
| F000'          | 1022.19          |                  |
| h,k,lmax       | 16,17,21         | 15,17,20         |
| Nref           | 11980            | 10800            |
| Tmin,Tmax      | 0.943,0.980      | 0.947,0.983      |
| Tmin'          | 0.904            |                  |

Correction method= GAUSSIAN

Data completeness= 0.902

Theta(max)= 27.500

R(reflections)= 0.0689( 4911)

wR2(reflections)= 0.1457( 10800)

S = 0.852

Npar= 613

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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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### [IMAGE] Alert level A

|  |   |
|--|---|
| PLAT901_ALERT_1_A Cell Parameters in CIF and FCF do not Match .... | ! |
| PLAT901_ALERT_1_A Cell Parameters in CIF and FCF do not Match .... | ! |
| PLAT902_ALERT_1_A No (Interpretable) Reflections found in FCF .... | ! |

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**[IMAGE] Alert level C**

|                   |   |       |        |       |
|-------------------|---|-------|--------|-------|
| PLAT026_ALERT_3_C | Ratio Observed / Unique Reflections too Low | ....  | 45     | Perc. |
| PLAT220_ALERT_2_C | Large Non-Solvent C Ueq(max)/Ueq(min)       | ...   | 3.4    | Ratio |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C24 -- C25       | ..    | 0.16   | Ang.  |
| PLAT342_ALERT_3_C | Low Bond Precision on C-C Bonds             | ..... | 0.0094 | Ang   |

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**[IMAGE] Alert level G**

|                   |  |      |      |      |
|-------------------|--|------|------|------|
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained Atom Sites    | .... | 2    |      |
| PLAT005_ALERT_5_G | No _iucr_refine_instructions_details in CIF    | .... | ?    |      |
| PLAT371_ALERT_2_G | Long C(sp2)-C(sp1) Bond C5 - C52               | ...  | 1.43 | Ang. |
| PLAT605_ALERT_4_G | Structure Contains Solvent Accessible VOIDS of | .    | 386  | A**3 |

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**Author Response: Two peaks were observed in later difference maps. From the reaction conditions, it would appear to be not sensible to model these as water molecules. Attempts to model this as any of the more likely solvents were unsuccessful. Hence the program Squeeze was used to effectively remove the electron density due to solvent molecules.**

|                   |   |       |    |  |
|-------------------|---|-------|----|--|
| PLAT860_ALERT_3_G | Note: Number of Least-Squares Restraints        | ..... | 12 |  |
| PLAT869_ALERT_4_G | ALERTS Related to the use of SQUEEZE Suppressed |       | !  |  |

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

3 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  
3 ALERT type 3 Indicator that the structure quality may be low  
3 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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## Datablock: br1511

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Bond precision: C-C = 0.0043 A

Wavelength=0.71073

|              |                  |                 |                 |
|--------------|------------------|-----------------|-----------------|
| Cell:        | a=10.9993(5)     | b=14.9920(7)    | c=16.4501(7)    |
|              | alpha=106.606(4) | beta=108.940(4) | gamma=95.089(4) |
| Temperature: | 100 K            |                 |                 |

|                | Calculated       | Reported         |
|----------------|------------------|------------------|
| Volume         | 2409.0(2)        | 2409.0(2)        |
| Space group    | P -1             | P -1             |
| Hall group     | -P 1             | -P 1             |
| Moiety formula | C54 H39 N3 P2 Ru | C54 H39 N3 P2 Ru |
| Sum formula    | C54 H39 N3 P2 Ru | C54 H39 N3 P2 Ru |
| Mr             | 892.89           | 892.89           |
| Dx,g cm-3      | 1.231            | 1.231            |
| Z              | 2                | 2                |
| Mu (mm-1)      | 0.429            | 0.429            |
| F000           | 916.0            | 916.0            |
| F000'          | 914.15           |                  |
| h,k,lmax       | 16,22,24         | 16,21,24         |
| Nref           | 16917            | 15503            |
| Tmin,Tmax      | 0.940,0.987      | 0.868,0.986      |
| Tmin'          | 0.773            |                  |

Correction method= ANALYTICAL

Data completeness= 0.916

Theta(max)= 32.130

R(reflections)= 0.0515( 9815)

wR2(reflections)= 0.1212( 15503)

S = 0.923

Npar= 586

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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[IMAGE] **Alert level B**

|  |           |
|--|-----------|
| PLAT910_ALERT_3_B Missing # of FCF Reflections Below Th(Min) ..... | 13        |
| PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ... | 1         |
| PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW .gt. 10 Outliers . | 8         |
| PLAT973_ALERT_2_B Large Calcd. Positive Residual Density on Rul    | 1.80 eA-3 |

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[IMAGE] **Alert level C**

|  |           |
|--|-----------|
| PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ...        | 3.2 Ratio |
| PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond C2 - C3 ...            | 1.37 Ang. |
| PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600  | 2         |
| PLAT912_ALERT_4_C Missing # of FCF Reflections Above STh/L= 0.600  | 1364      |
| PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... | 1         |
| PLAT918_ALERT_3_C Reflection(s) # with I(obs) much smaller I(calc) | 1         |

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[IMAGE] **Alert level G**

|  |              |
|--|--------------|
| PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite | 12           |
| PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites .... | 11           |
| PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... | ?            |
| PLAT154_ALERT_1_G The su's on the Cell Angles are Equal .....      | 0.00400 Deg. |
| PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Rul -- C1 ..           | 7.1 su       |
| PLAT301_ALERT_3_G Note: Main Residue Disorder .....                | 18 Perc.     |
| PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of . | 413 A**3     |

PLAT811\_ALERT\_5\_G No ADDSYM Analysis: Too Many Excluded Atoms .... !  
 PLAT860\_ALERT\_3\_G Note: Number of Least-Squares Restraints ..... 126  
 PLAT869\_ALERT\_4\_G ALERTS Related to the use of SQUEEZE Suppressed !  
 PLAT961\_ALERT\_5\_G Dataset Contains no Negative Intensities ..... !

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 11 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 6 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 8 ALERT type 3 Indicator that the structure quality may be low  
 3 ALERT type 4 Improvement, methodology, query or suggestion  
 3 ALERT type 5 Informative message, check

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## Datablock: br1517b

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Bond precision: C-C = 0.0043 A Wavelength=0.71073

Cell: a=13.6841(5) b=15.1893(5) c=18.9302(8)  
 alpha=84.010(3) beta=88.044(3) gamma=69.523(3)

Temperature: 100 K

|                | Calculated                      | Reported                        |
|----------------|---------------------------------|---------------------------------|
| Volume         | 3665.9(2)                       | 3665.9(2)                       |
| Space group    | P -1                            | P -1                            |
| Hall group     | -P 1                            | -P 1                            |
| Moiety formula | 4(C43 H29 N4 P Ru), 3(C H2 Cl2) | C43 H29 N4 P Ru, 0.75(C H2 Cl2) |
| Sum formula    | C175 H122 Cl6 N16 P4 Ru4        | C43.75 H30.50 Cl1.50 N4 P Ru    |
| Mr             | 3189.75                         | 797.44                          |
| Dx,g cm-3      | 1.445                           | 1.445                           |
| Z              | 1                               | 4                               |
| Mu (mm-1)      | 0.618                           | 0.618                           |
| F000           | 1622.0                          | 1622.0                          |
| F000'          | 1618.69                         |                                 |
| h,k,lmax       | 20,23,28                        | 20,22,28                        |
| Nref           | 27003                           | 24229                           |
| Tmin,Tmax      | 0.843,0.982                     | 0.840,0.980                     |
| Tmin'          | 0.762                           |                                 |

Correction method= ANALYTICAL

Data completeness= 0.897 Theta(max)= 32.720

R(reflections)= 0.0490( 14415) wR2(reflections)= 0.1185( 24229)

S = 0.908

Npar= 1045

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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[IMAGE] **Alert level B**

|  |           |
|--|-----------|
| PLAT910_ALERT_3_B Missing # of FCF Reflections Below Th(Min) ..... | 43        |
| PLAT971_ALERT_2_B Large Calcd. Non-Metal Positive Residual Density | 2.68 eA-3 |

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[IMAGE] **Alert level C**

|   |             |
|---|-------------|
| PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ   | ?           |
| PLAT045_ALERT_1_C Calculated and Reported Z Differ by .....         | 0.25 Ratio  |
| PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ...         | 3.2 Ratio   |
| PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C20 |             |
| PLAT245_ALERT_2_C U(iso) H133 Smaller than U(eq) C153 by ...        | 0.012 AngSq |
| PLAT245_ALERT_2_C U(iso) H134 Smaller than U(eq) C154 by ...        | 0.012 AngSq |
| PLAT245_ALERT_2_C U(iso) H136 Smaller than U(eq) C156 by ...        | 0.023 AngSq |
| PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....  | 2.5         |
| PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond C3 - C31 ...            | 1.36 Ang.   |
| PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond C6 - C61 ...            | 1.38 Ang.   |
| PLAT411_ALERT_2_C Short Inter H...H Contact H35 .. H144 ..          | 2.08 Ang.   |
| PLAT912_ALERT_4_C Missing # of FCF Reflections Above STh/L= 0.600   | 2711        |
| PLAT971_ALERT_2_C Large Calcd. Non-Metal Positive Residual Density  | 2.48 eA-3   |
| PLAT971_ALERT_2_C Large Calcd. Non-Metal Positive Residual Density  | 2.18 eA-3   |
| PLAT972_ALERT_2_C Large Calcd. Non-Metal Negative Residual Density  | -2.09 eA-3  |
| PLAT972_ALERT_2_C Large Calcd. Non-Metal Negative Residual Density  | -2.07 eA-3  |
| PLAT972_ALERT_2_C Large Calcd. Non-Metal Negative Residual Density  | -2.01 eA-3  |
| PLAT972_ALERT_2_C Large Calcd. Non-Metal Negative Residual Density  | -1.93 eA-3  |

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[IMAGE] **Alert level G**

|  |              |
|--|--------------|
| PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... | ?            |
| PLAT154_ALERT_1_G The su's on the Cell Angles are Equal .....      | 0.00300 Deg. |
| PLAT301_ALERT_3_G Note: Main Residue Disorder .....                | 12 Perc.     |
| PLAT302_ALERT_4_G Note: Anion/Solvent Disorder .....               | 33 Perc.     |
| PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C340 - C341 ...          | 1.43 Ang.    |
| PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C340 - C342 ...          | 1.43 Ang.    |
| PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C640 - C641 ...          | 1.43 Ang.    |
| PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C640 - C642 ...          | 1.42 Ang.    |
| PLAT432_ALERT_2_G Short Inter X...Y Contact C111 .. C134 ..        | 2.96 Ang.    |

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- |    |   |
|----|---|
| 0  | <b>ALERT level A</b> = Most likely a serious problem - resolve or explain         |
| 2  | <b>ALERT level B</b> = A potentially serious problem, consider carefully          |
| 18 | <b>ALERT level C</b> = Check. Ensure it is not caused by an omission or oversight |
| 9  | <b>ALERT level G</b> = General information/check it is not something unexpected   |
| 3  | <b>ALERT type 1</b> CIF construction/syntax error, inconsistent or missing data   |
| 20 | <b>ALERT type 2</b> Indicator that the structure model may be wrong or deficient  |
| 2  | <b>ALERT type 3</b> Indicator that the structure quality may be low               |
| 3  | <b>ALERT type 4</b> Improvement, methodology, query or suggestion                 |
| 1  | <b>ALERT type 5</b> 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*, 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.

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**PLATON version of 21/12/2011; check.def file version of 16/12/2011**

### **Datablock br1425 - ellipsoid plot**

[IMAGE]

### **Datablock br1511 - ellipsoid plot**

[IMAGE]

### **Datablock br1517b - ellipsoid plot**

[IMAGE]