

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

| | | | |
|-----------------|----------------|--------------------|---------------|
| Bond precision: | C-C = 0.0041 A | Wavelength=0.71073 | |
| Cell: | a=10.0271 (5) | b=9.9616 (5) | c=15.4734 (6) |
| | alpha=90 | beta=107.260 (2) | gamma=90 |
| Temperature: | 150 K | | |

```
Correction method= # Reported T Limits: Tmin=0.810 Tmax=0.930
AbsCorr = MULTI-SCAN
```

| | |
|-------------------------------|---------------------------------|
| R(reflections)= 0.0259(2176) | wR2(reflections)= 0.0614(2686) |
| S = 1.062 | Npar= 180 |

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 C

| | | | | | | | |
|-------------------|------------|--------|---|---------------------|-------|-----|-------|
| PLAT220_ALERT_2_C | NonSolvent | Resd 1 | C | Ueq(max)/Ueq(min) | Range | 3.5 | Ratio |
| PLAT222_ALERT_3_C | NonSolvent | Resd 1 | H | Uiso(max)/Uiso(min) | Range | 4.1 | Ratio |



Alert level G

| | | | | | |
|-------------------|--|-----|---|--------|------|
| PLAT333_ALERT_2_G | Large Aver C6-Ring C-C Dist C1 | -C6 | . | 1.42 | Ang. |
| PLAT883_ALERT_1_G | No Info/Value for _atom_sites_solution_primary | . | | Please | Do ! |
| PLAT933_ALERT_2_G | Number of HKL-OMIT Records in Embedded .res File | | | 6 | Note |
| | 0 0 2, 1 1 0, 0 1 1, 1 0 0, -1 0 2, -1 1 1, | | | | |

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

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

Datablock: 03646

Bond precision: C-C = 0.0153 A

Wavelength=0.71073

| | | | |
|-------|-------------|-------------|-------------|
| Cell: | a=11.204(3) | b=11.914(4) | c=18.984(5) |
| | alpha=90 | beta=90 | gamma=90 |

Temperature: 150 K

| | Calculated | Reported |
|------------------------|------------------------|-----------------------|
| Volume | 2534.1(13) | 2534.1(13) |
| Space group | P 21 21 21 | P 21 21 21 |
| Hall group | P 2ac 2ab | P 2ac 2ab |
| Moiety formula | C25 H24 Cl N2 Ru, F6 P | ? |
| Sum formula | C25 H24 Cl F6 N2 P Ru | C25 H24 Cl F6 N2 P Ru |
| Mr | 633.95 | 633.95 |
| Dx, g cm ⁻³ | 1.662 | 1.662 |
| Z | 4 | 4 |
| Mu (mm ⁻¹) | 0.849 | 0.849 |
| F000 | 1272.0 | 1272.0 |
| F000' | 1268.60 | |
| h,k,lmax | 13,14,22 | 13,14,22 |
| Nref | 4629[2627] | 4588 |
| Tmin,Tmax | 0.915,0.963 | 0.770,0.960 |
| Tmin' | 0.866 | |

Correction method= # Reported T Limits: Tmin=0.770 Tmax=0.960
AbsCorr = MULTI-SCAN

Data completeness= 1.75/0.99 Theta(max)= 25.310

R(reflections)= 0.0463(3581) wR2(reflections)=
0.1195(4588)
S = 1.029 Npar= 327

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 C

| | | | | | | | |
|-------------------|--|-----------|---------------------------------|-------------------|-------|---------|-------|
| PLAT220_ALERT_2_C | NonSolvent | Resd 1 | C | Ueq(max)/Ueq(min) | Range | 3.5 | Ratio |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | P1 | --F6 | . | | 0.16 | Ang. |
| PLAT242_ALERT_2_C | Low | 'MainMol' | Ueq as Compared to Neighbors of | | | C7 | Check |
| PLAT242_ALERT_2_C | Low | 'MainMol' | Ueq as Compared to Neighbors of | | | C13 | Check |
| PLAT250_ALERT_2_C | Large U3/U1 Ratio for <U(i,j)> Tensor | (Resd 2) | | | | 2.1 | Note |
| PLAT260_ALERT_2_C | Large Average Ueq of Residue Including | P1 | | | | 0.110 | Check |
| PLAT342_ALERT_3_C | Low Bond Precision on C-C Bonds | | | | | 0.01532 | Ang. |
| PLAT360_ALERT_2_C | Short C(sp3)-C(sp3) Bond | C13 | - C15 | . | | 1.41 | Ang. |

● Alert level G

| | | | |
|-------------------|--|-----|-------------|
| PLAT187_ALERT_4_G | The CIF-Embedded .res File Contains RIGU Records | 1 | Report |
| PLAT244_ALERT_4_G | Low 'Solvent' Ueq as Compared to Neighbors of | P1 | Check |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints | 355 | Note |
| PLAT883_ALERT_1_G | No Info/Value for _atom_sites_solution_primary | | Please Do ! |
| PLAT933_ALERT_2_G | Number of HKL-OMIT Records in Embedded .res File | 9 | Note |
| | 0 2 1, 0 2 0, 1 1 0, 1 0 1, 0 0 2, 0 1 1, | | |

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

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

Datablock: 03612

Bond precision: C-C = 0.0040 Å Wavelength=1.54184

Cell: a=10.3217(1) b=16.4107(2) c=9.6932(1)
alpha=90 beta=103.179(1) gamma=90

Temperature: 150 K

| | Calculated | Reported |
|------------------------|------------------|------------------|
| Volume | 1598.65(3) | 1598.65(3) |
| Space group | P 21/c | P 1 21/c 1 |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C18 H17 Cl2 N Ru | C18 H17 Cl2 N Ru |
| Sum formula | C18 H17 Cl2 N Ru | C18 H17 Cl2 N Ru |
| Mr | 419.30 | 419.29 |
| Dx, g cm ⁻³ | 1.742 | 1.742 |
| Z | 4 | 4 |
| Mu (mm ⁻¹) | 10.955 | 10.955 |
| F000 | 840.0 | 840.0 |
| F000' | 844.69 | |
| h,k,lmax | 12,19,11 | 12,19,11 |
| Nref | 2927 | 2926 |
| Tmin,Tmax | 0.566,0.936 | 0.556,0.967 |
| Tmin' | 0.433 | |

Correction method= # Reported T Limits: Tmin=0.556 Tmax=0.967
AbsCorr = GAUSSIAN

Data completeness= 1.000 Theta(max)= 68.284

R(reflections)= 0.0236(2662)

wR2(reflections)=
0.0565(2926)

S = 1.050

Npar= 201

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 G

PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C1 -C6 . 1.42 Ang.

-
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0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
1 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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0 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
-

Datablock: 03632

Bond precision: C-C = 0.0051 A

Wavelength=0.71073

Cell: a=17.5378(9) b=8.9998(6) c=19.7552(12)
alpha=90 beta=108.763(2) gamma=90

Temperature: 150 K

| | Calculated | Reported |
|------------------------|-------------------------|----------------------|
| Volume | 2952.4 (3) | 2952.4 (3) |
| Space group | P 21/c | P 1 21/c 1 |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C28 H25 N3 Ru, 2 (F6 P) | ? |
| Sum formula | C28 H25 F12 N3 P2 Ru | C28 H25 F12 N3 P2 Ru |
| Mr | 794.52 | 794.52 |
| Dx, g cm ⁻³ | 1.788 | 1.787 |
| Z | 4 | 4 |
| Mu (mm ⁻¹) | 0.742 | 0.742 |
| F000 | 1584.0 | 1584.0 |
| F000' | 1580.83 | |
| h, k, lmax | 21, 10, 23 | 21, 10, 23 |
| Nref | 5409 | 5392 |
| Tmin, Tmax | 0.884, 0.975 | 0.860, 0.970 |
| Tmin' | 0.825 | |

Correction method= # Reported T Limits: Tmin=0.860 Tmax=0.970
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 25.350

R(reflections)= 0.0372 (4217) wR2(reflections)=
0.0848 (5392)
S = 1.022 Npar= 417

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 G

| | | |
|--|---|-------------|
| PLAT244_ALERT_4_G Low | 'Solvent' Ueq as Compared to Neighbors of | P1 Check |
| PLAT244_ALERT_4_G Low | 'Solvent' Ueq as Compared to Neighbors of | P2 Check |
| PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . | | Please Do ! |
| PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File | | 11 Note |
| 0 0 2, | 0 1 1, -1 0 2, -1 1 1, -2 0 2, | 1 1 0, |
| 1 1 1, | 2 0 0, 0 1 2, 1 0 2, -1 1 2, | |

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- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

1 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: 03654

Bond precision: C-C = 0.0052 Å Wavelength=0.71073
Cell: a=17.6681(6) b=9.0053(4) c=19.7826(6)
alpha=90 beta=109.248(1) gamma=90
Temperature: 150 K

| | Calculated | Reported |
|------------------------|------------------------|----------------------|
| Volume | 2971.60(19) | 2971.60(19) |
| Space group | P 21/c | P 1 21/c 1 |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C28 H25 N3 Os, 2(F6 P) | ? |
| Sum formula | C28 H25 F12 N3 Os P2 | C28 H25 F12 N3 Os P2 |
| Mr | 883.68 | 883.65 |
| Dx, g cm ⁻³ | 1.975 | 1.975 |
| Z | 4 | 4 |
| Mu (mm ⁻¹) | 4.501 | 4.501 |
| F000 | 1712.0 | 1712.0 |
| F000' | 1709.12 | |
| h,k,lmax | 21,10,23 | 21,10,23 |
| Nref | 5425 | 5414 |
| Tmin,Tmax | 0.605,0.806 | 0.620,0.810 |
| Tmin' | 0.427 | |

Correction method= # Reported T Limits: Tmin=0.620 Tmax=0.810
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 25.330

R(reflections)= 0.0218(5037) wR2(reflections)=
0.0520(5414)
S = 1.095 Npar= 481

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.

PLAT094 ALERT 2 C Ratio of Maximum / Minimum Residual Density 2.25 Report

| | | | |
|-------------------|--|------|-------------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | 14 | Note |
| PLAT003_ALERT_2_G | Number of Uiso or U(i,j) Restrained non-H Atoms | 14 | Report |
| PLAT083_ALERT_2_G | SHELXL Second Parameter in WGHT Unusually Large | 6.90 | Why ? |
| PLAT172_ALERT_4_G | The CIF-Embedded .res File Contains DFIX Records | 2 | Report |
| PLAT173_ALERT_4_G | The CIF-Embedded .res File Contains DANG Records | 10 | Report |
| PLAT177_ALERT_4_G | The CIF-Embedded .res File Contains DELU Records | 2 | Report |
| PLAT178_ALERT_4_G | The CIF-Embedded .res File Contains SIMU Records | 2 | Report |
| PLAT187_ALERT_4_G | The CIF-Embedded .res File Contains RIGU Records | 2 | Report |
| PLAT244_ALERT_4_G | Low 'Solvent' Ueq as Compared to Neighbors of | P2 | Check |
| PLAT302_ALERT_4_G | Anion/Solvent/Minor-Residue Disorder (Resd 2) | 100% | Note |
| PLAT302_ALERT_4_G | Anion/Solvent/Minor-Residue Disorder (Resd 4) | 100% | Note |
| PLAT304_ALERT_4_G | Non-Integer Number of Atoms in (Resd 2) | 5.61 | Check |
| PLAT304_ALERT_4_G | Non-Integer Number of Atoms in (Resd 4) | 1.39 | Check |
| PLAT333_ALERT_2_G | Large Aver C6-Ring C-C Dist C1 -C6 . | 1.42 | Ang. |
| PLAT432_ALERT_2_G | Short Inter X...Y Contact F5B ..C25 . | 2.96 | Ang. |
| | x,y,z = 1_555 | | Check |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints | 276 | Note |
| PLAT883_ALERT_1_G | No Info/Value for _atom_sites_solution_primary . | | Please Do ! |
| PLAT933_ALERT_2_G | Number of HKL-OMIT Records in Embedded .res File | 9 | Note |
| | -2 0 2, -1 1 1, 1 1 1, -1 0 2, 1 1 0, 2 0 0, | | |
| | 1 0 2, 0 1 1, 0 0 2, | | |

| | | |
|----|----------------------|--|
| 0 | ALERT level A | = Most likely a serious problem - resolve or explain |
| 0 | ALERT level B | = A potentially serious problem, consider carefully |
| 1 | ALERT level C | = Check. Ensure it is not caused by an omission or oversight |
| 18 | ALERT level G | = General information/check it is not something unexpected |

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1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
10 ALERT type 4 Improvement, methodology, query or suggestion
0 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.









