Datablock: 2

Bond precision: \( C-C = 0.0103 \) \( \text{A} \) \hspace{1cm} \text{Wavelength}=0.71073

Cell:
\[
\begin{align*}
\text{a} &= 16.8737(3) \\
\text{b} &= 14.6964(6) \\
\text{c} &= 22.3909(7) \\
\alpha &= 90 \\
\beta &= 90 \\
\gamma &= 90
\end{align*}
\]

Temperature: \( 150 \text{ K} \)

Volume \hspace{1cm} \text{Calculated} \hspace{1cm} \text{Reported}
\[
5552.6(3) \hspace{1cm} 5552.6(3)
\]

Space group \hspace{1cm} \text{P b c a} \hspace{1cm} \text{P b c a}

Hall group \hspace{1cm} \text{-P 2ac 2ab} \hspace{1cm} \text{-P 2ac 2ab}

Moiety formula
\[
\text{C21 H28 N3 Ru, C4 H8 O, F6 P}
\]

Sum formula
\[
\text{C25 H36 F6 N3 O P Ru}
\]

Mr \hspace{1cm} 640.61 \hspace{1cm} 640.61

Dx,g cm\(^{-3}\) \hspace{1cm} 1.533 \hspace{1cm} 1.533

Z \hspace{1cm} 8 \hspace{1cm} 8

Mu (mm\(^{-1}\)) \hspace{1cm} 0.686 \hspace{1cm} 0.686

F000 \hspace{1cm} 2624.0 \hspace{1cm} 2624.0

F000’ \hspace{1cm} 2616.08

h,k,lmax \hspace{1cm} 20,17,26 \hspace{1cm} 20,17,26

Nref \hspace{1cm} 4893 \hspace{1cm} 4879

Tmin,Tmax \hspace{1cm} 0.906,0.947 \hspace{1cm} 0.828,0.960

Correction method= MULTI-SCAN

Data completeness= 0.997 \hspace{2cm} \text{Theta(max)}= 25.000

R(reflections)= 0.0568( 2958) \hspace{1cm} \text{wR2(reflections)}= 0.1800( 4879)

S = 1.038 \hspace{2cm} \text{Npar}= 342

The following ALERTS were generated. Each ALERT has the format
\text{test-name_ALERT_alert-type_alert-level}.
Click on the hyperlinks for more details of the test.

\begin{tabular}{|l|l|}
\hline
\textbf{Alert level C} & \\
\hline
PLAT094_ALERT_2_C & Ratio of Maximum / Minimum Residual Density .... 2.47 \\
PLAT250_ALERT_2_C & Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.99 \\
PLAT342_ALERT_3_C & Low Bond Precision on C-C Bonds (x 1000) Ang .. 10 \\
PLAT360_ALERT_2_C & Short C(sp3)-C(sp3) Bond C1S - C2S ... 1.41 Ang. \\
PLAT042_ALERT_1_C & Calc. and Reported MoietyFormula Strings Differ ? \\
\hline
\end{tabular}
<table>
<thead>
<tr>
<th>Alert</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>G</td>
<td>General alerts; check</td>
</tr>
<tr>
<td>A</td>
<td>In general: serious problem</td>
</tr>
<tr>
<td>B</td>
<td>Potentially serious problem</td>
</tr>
<tr>
<td>C</td>
<td>Check and explain</td>
</tr>
<tr>
<td>G</td>
<td>SHELXL Second Parameter in WHT Unusually Large. 8.55</td>
</tr>
<tr>
<td>G</td>
<td>Number of Unusual/Non-Standard Labels .......... 9</td>
</tr>
</tbody>
</table>

**Datablock: 6**

**Bond precision:** C-C = 0.0167 A  
**Wavelength:** 0.71073

**Cell:**  
\[ a=12.7810(15) \quad b=16.890(2) \quad c=13.5646(16) \]  
\[ \alpha=90 \quad \beta=113.406(9) \quad \gamma=90 \]

**Temperature:** 150 K

**Volume:**  
Calculated: 2687.3(6)  
Reported: 2687.3(6)

**Space group:**  
P 21/n  
P 21/n

**Hall group:**  
-P 2yn  
-P 2yn

**Moiety formula:**  
C21 H27 Cl N3 Os, F6 P

**Sum formula:**  
C21 H27 Cl F6 N3 Os P

**Mr:** 692.11  
692.08

**Dx, g cm\(^{-3}\):** 1.711  
1.711

**Z:** 4  
4

**Mu (mm\(^{-1}\):** 4.959  
4.959

**F000:** 1344.0  
1344.0

**F000':** 1340.93

**h,k,lmax:** 15,20,16  
15,20,15

**Nref:** 4731  
4338

**Tmin,Tmax:** 0.627,0.906  
0.437,0.907

**Tmin':** 0.367

**Correction method:** MULTI-SCAN

**Data completeness:** 0.917  
**Theta(max):** 25.000
The following ALERTS were generated. Each ALERT has the format
\texttt{test-name\_ALERT\_alert-type\_alert-level}.
Click on the hyperlinks for more details of the test.

**Alert level A**

\texttt{PLAT029\_ALERT\_3\_A} \_dифfrn\_measured\_fraction\_theta\_full Low \ldots \ldots \ 0.92

**Alert level B**

\texttt{PLAT601\_ALERT\_2\_B} Structure Contains Solvent Accessible VOIDS of . 199.00 A**3

**Alert level C**

\texttt{REFT03\_ALERT\_3\_C} Reflection count < 95% complete

From the CIF: \_dифfrn\_refl\_s\_theta\_max 25.00
From the CIF: \_dифfrn\_refl\_s\_theta\_full 25.00
From the CIF: \_refl\_number\_total 4338

TEST2: Refl\_s within \_dифfrn\_refl\_s\_theta\_max
Count of symmetry unique refl\_s 4731
Completeness (\_total/calc) 91.69%

\texttt{RINTA01\_ALERT\_3\_C} The value of Rint is greater than 0.12

Rint given 0.166

\texttt{PLAT022\_ALERT\_3\_C} Ratio Unique / Expected Reflections too Low .... 0.92

\texttt{PLAT250\_ALERT\_2\_C} Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.44

\texttt{PLAT342\_ALERT\_3\_C} Low Bond Precision on C-C Bonds (x 1000) Ang .. 17

\texttt{PLAT420\_ALERT\_2\_C} D-H Without Acceptor N3 - H3B ... ?

\texttt{PLAT234\_ALERT\_4\_C} Large Hirshfeld Difference C8 -- C9 .. 0.23 Ang.

\texttt{PLAT234\_ALERT\_4\_C} Large Hirshfeld Difference C12 -- C13 .. 0.20 Ang.

\texttt{PLAT234\_ALERT\_4\_C} Large Hirshfeld Difference C16 -- C17 .. 0.17 Ang.

\texttt{PLAT234\_ALERT\_4\_C} Large Hirshfeld Difference C19 -- C21 .. 0.18 Ang.

\texttt{PLAT244\_ALERT\_4\_C} Low 'Solvent' Ueq as Compared to Neighbors of P3

\texttt{PLAT732\_ALERT\_1\_C} Angle Calc 37.5(3), Rep 37.49(11) .... 2.73 su-Ra

C17 - O51 - C12 1.555 1.555 1.555 # 6

\texttt{PLAT732\_ALERT\_1\_C} Angle Calc 37.4(3), Rep 37.32(11) .... 2.73 su-Ra

C17 - O51 - C16 1.555 1.555 1.555 # 9

\texttt{PLAT732\_ALERT\_1\_C} Angle Calc 37.3(3), Rep 37.30(10) .... 3.00 su-Ra

C12 - O51 - C13 1.555 1.555 1.555 # 14

\texttt{PLAT732\_ALERT\_1\_C} Angle Calc 79.1(3), Rep 79.13(14) .... 2.14 su-Ra

C16 - O51 - C13 1.555 1.555 1.555 # 15

\texttt{PLAT732\_ALERT\_1\_C} Angle Calc 36.9(3), Rep 36.98(9) .... 3.33 su-Ra

C16 - O51 - C15 1.555 1.555 1.555 # 20

\texttt{PLAT732\_ALERT\_1\_C} Angle Calc 79.1(3), Rep 79.13(14) .... 2.14 su-Ra

C17 - O51 - C14 1.555 1.555 1.555 # 24

\texttt{PLAT732\_ALERT\_1\_C} Angle Calc 66.6(3), Rep 66.63(13) .... 2.31 su-Ra

C16 - O51 - C14 1.555 1.555 1.555 # 26

\texttt{PLAT732\_ALERT\_1\_C} Angle Calc 36.8(3), Rep 36.80(9) .... 3.33 su-Ra

C15 - O51 - C14 1.555 1.555 1.555 # 28

\texttt{PLAT732\_ALERT\_1\_C} Angle Calc 70.6(5), Rep 70.6(2) .... 2.50 su-Ra

C12 - C13 - O51 1.555 1.555 1.555 # 67

\texttt{PLAT790\_ALERT\_4\_C} Centre of Gravity not Within Unit Cell: Resd. # 2
1 ALERT level A = In general: serious problem
1 ALERT level B = Potentially serious problem
2 ALERT level C = Check and explain
1 ALERT level G = General alerts; check

9 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
5 ALERT type 3 Indicator that the structure quality may be low
7 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be taken off CIFs submitted for publication in IUCr journals (Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation); however, if you intend to submit your CIF to Acta Crystallographica Section C or E, you should make sure that the 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.

Datablock 2 - ellipsoid plot

Datablock 6 - ellipsoid plot