

No syntax errors found.  
Please wait while processing ....

[CIF dictionary](#)  
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## Datablock: mo\_aaa\_fr\_0m

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Bond precision: C-C = 0.0066 A Wavelength=0.71073  
Cell: a=9.5483(2) b=11.6728(2) c=40.0824(8)  
alpha=90 beta=95.371(1) gamma=90  
Temperature 302 K  
:  
Calculated Reported  
Volume 4447.79(15) 4447.79(15)  
Space group P 21/c P 1 21/c 1  
Hall group -P 2ybc -P 2ybc  
Moiety formula C32 H43 N3 O P2 Ru S, 2(C F3 O3C32 H43 N3 O P2 Ru S, 2(C F3 O3  
S), C3 H6 O S), C3 H6 O  
Sum formula C37 H49 F6 N3 O8 P2 Ru S3 C37 H49 F6 N3 O8 P2 Ru S3  
Mr 1036.98 1036.98  
Dx,g cm-3 1.549 1.549  
Z 4 4  
Mu (mm-1) 0.642 0.642  
F000 2128.0 2128.0  
F000' 2126.34  
h,k,lmax 14,17,58 14,17,58  
Nref 14789 14781  
Tmin,Tmax 0.781,0.825 0.066,0.102  
Tmin' 0.766  
Correction method= # Reported T Limits: Tmin=0.066  
Tmax=0.102 AbsCorr = MULTI-SCAN  
Data completeness= 0.999 Theta(max)= 31.506  
R(reflections)= 0.0622( 11828) wR2(reflections)=  
0.1620( 14781)  
S = 1.061 Npar= 551

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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 C

|                                   |  |   |       |        |
|-----------------------------------|--|---|-------|--------|
| <a href="#">PLAT241_ALERT_2_C</a> | High   | 'MainMol' Ueq as Compared to Neighbors of | C16   | Check  |
| <a href="#">PLAT242_ALERT_2_C</a> | Low  | 'MainMol' Ueq as Compared to Neighbors of | Ru1   | Check  |
| <a href="#">PLAT244_ALERT_4_C</a> | Low  | 'Solvent' Ueq as Compared to Neighbors of | S1T   | Check  |
| <a href="#">PLAT244_ALERT_4_C</a> | Low  | 'Solvent' Ueq as Compared to Neighbors of | C2A   | Check  |
| <a href="#">PLAT260_ALERT_2_C</a> | Large Average Ueq of Residue Including           | S1T                                       | 0.113 | Check  |
| <a href="#">PLAT906_ALERT_3_C</a> | Large K Value in the Analysis of Variance .....  |   | 6.427 | Check  |
| <a href="#">PLAT911_ALERT_3_C</a> | Missing FCF Refl Between Thmin & STh/L=          | 0.600                                     | 6     | Report |
| <a href="#">PLAT913_ALERT_3_C</a> | Missing # of Very Strong Reflections in FCF .... |   | 4     | Note   |
| <a href="#">PLAT976_ALERT_2_C</a> | Check Calcd Resid. Dens.                         | 0.47Ang From O5TA                         | -0.54 | eA-3   |

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### Alert level G

|                                   |  |               |      |        |
|-----------------------------------|--|---------------|------|--------|
| <a href="#">PLAT007_ALERT_5_G</a> | Number of Unrefined Donor-H Atoms .....          |               | 1    | Report |
| <a href="#">PLAT083_ALERT_2_G</a> | SHELXL Second Parameter in WGHT Unusually Large  |               | 8.15 | Why ?  |
| <a href="#">PLAT171_ALERT_4_G</a> | The CIF-Embedded .res File Contains EADP Records |               | 5    | Report |
| <a href="#">PLAT187_ALERT_4_G</a> | The CIF-Embedded .res File Contains RIGU Records |               | 1    | Report |
| <a href="#">PLAT231_ALERT_4_G</a> | Hirshfeld Test (Solvent)                         | S2TA --O4TA . | 11.3 | s.u.   |

#### And 10 other PLAT231 Alerts

|                                   |                          |               |      |      |
|-----------------------------------|--------------------------|---------------|------|------|
| <a href="#">PLAT231_ALERT_4_G</a> | Hirshfeld Test (Solvent) | S2TA --O6TA . | 11.0 | s.u. |
| <a href="#">PLAT231_ALERT_4_G</a> | Hirshfeld Test (Solvent) | S2TA --O5TA . | 15.0 | s.u. |
| <a href="#">PLAT231_ALERT_4_G</a> | Hirshfeld Test (Solvent) | S2TB --C2T .  | 6.4  | s.u. |
| <a href="#">PLAT231_ALERT_4_G</a> | Hirshfeld Test (Solvent) | F4TA --C2T .  | 5.4  | s.u. |
| <a href="#">PLAT231_ALERT_4_G</a> | Hirshfeld Test (Solvent) | F6TA --C2T .  | 6.4  | s.u. |
| <a href="#">PLAT231_ALERT_4_G</a> | Hirshfeld Test (Solvent) | F5TA --C2T .  | 5.6  | s.u. |
| <a href="#">PLAT231_ALERT_4_G</a> | Hirshfeld Test (Solvent) | S1T --C1T .   | 6.2  | s.u. |
| <a href="#">PLAT231_ALERT_4_G</a> | Hirshfeld Test (Solvent) | F1T --C1T .   | 7.7  | s.u. |

|                                   |                          |     |       |   |           |
|-----------------------------------|--------------------------|-----|-------|---|-----------|
| <a href="#">PLAT231_ALERT_4_G</a> | Hirshfeld Test (Solvent) | F2T | --C1T | . | 9.2 s.u.  |
| <a href="#">PLAT231_ALERT_4_G</a> | Hirshfeld Test (Solvent) | F3T | --C1T | . | 14.0 s.u. |

|                                   |  |     |       |
|-----------------------------------|--|-----|-------|
| <a href="#">PLAT244_ALERT_4_G</a> | Low 'Solvent' Ueq as Compared to Neighbors of    | C1T | Check |
| <a href="#">PLAT302_ALERT_4_G</a> | Anion/Solvent/Minor-Residue Disorder (Resd 2 )   | 88% | Note  |
| <a href="#">PLAT720_ALERT_4_G</a> | Number of Unusual/Non-Standard Labels .....      | 20  | Note  |
| <a href="#">PLAT860_ALERT_3_G</a> | Number of Least-Squares Restraints .....         | 511 | Note  |
| <a href="#">PLAT910_ALERT_3_G</a> | Missing # of FCF Reflection(s) Below Theta(Min). | 2   | Note  |
| <a href="#">PLAT978_ALERT_2_G</a> | Number C-C Bonds with Positive Residual Density. | 0   | Info  |
| <a href="#">PLAT992_ALERT_5_G</a> | Repd & Actual _reflns_number_gt Values Differ by | 2   | Check |

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

0 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  
5 ALERT type 3 Indicator that the structure quality may be low  
18 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.

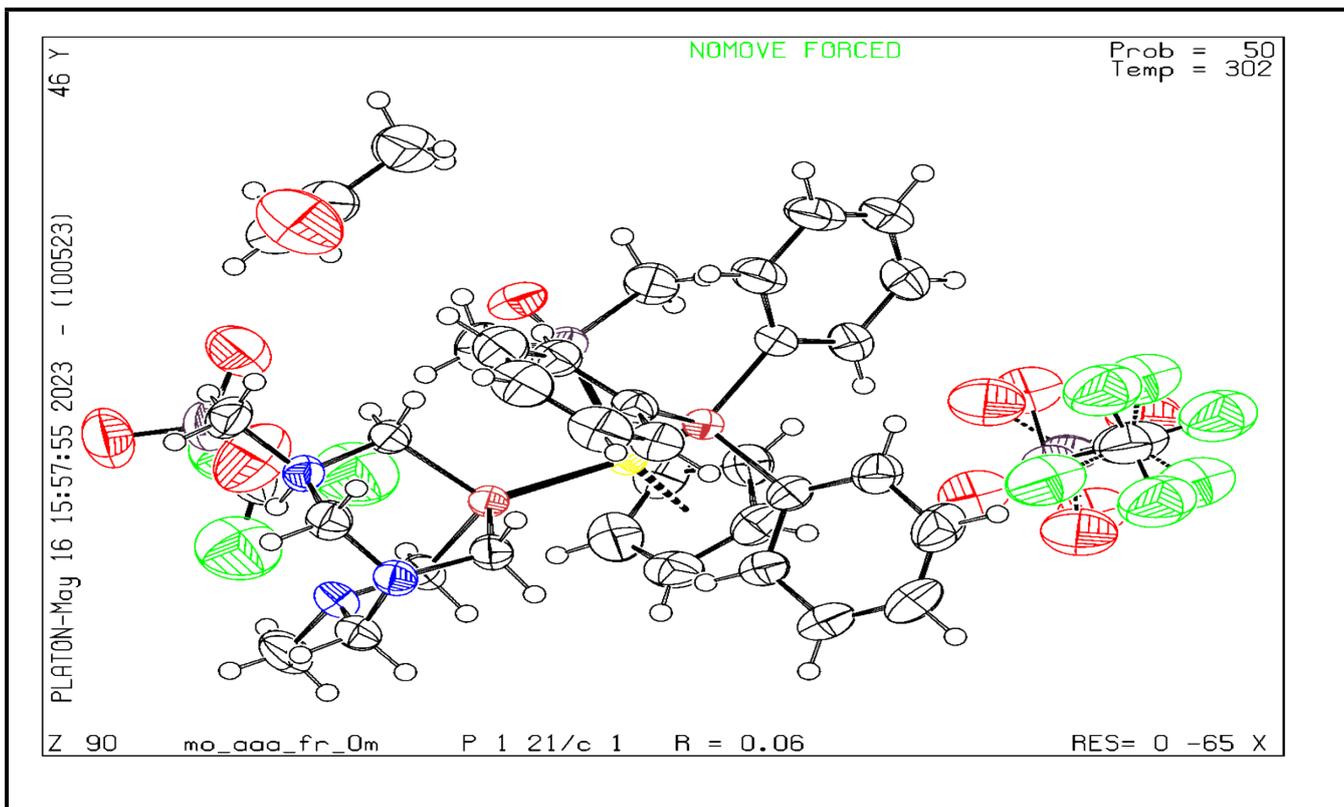
### Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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PLATON version of 10/05/2023; check.def file version of 10/05/2023

**Datablock mo\_aaa\_fr\_0m - ellipsoid plot**



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