

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kru519

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: kru519

Bond precision: C-C = 0.0046 Å Wavelength=0.71073

Cell: a=10.4158(2) b=10.8548(2) c=20.9285(4)
 alpha=99.831(1) beta=94.477(1) gamma=109.036(1)
Temperature: 173 K

| | Calculated | Reported |
|------------------------|----------------------------|----------------------------|
| Volume | 2181.12(7) | 2181.12(7) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C28 H38 Cl8 N10 Na2 O6 Ru2 | C28 H38 Cl8 N10 Na2 O6 Ru2 |
| Sum formula | C28 H38 Cl8 N10 Na2 O6 Ru2 | C28 H38 Cl8 N10 Na2 O6 Ru2 |
| Mr | 1142.41 | 1142.40 |
| Dx, g cm ⁻³ | 1.740 | 1.739 |
| Z | 2 | 2 |
| Mu (mm ⁻¹) | 1.254 | 1.254 |
| F000 | 1140.0 | 1140.0 |
| F000' | 1137.73 | |
| h, k, lmax | 16, 16, 32 | 16, 16, 32 |
| Nref | 16767 | 16301 |
| Tmin, Tmax | 0.900, 0.963 | 0.648, 0.747 |
| Tmin' | 0.778 | |

Correction method= # Reported T Limits: Tmin=0.648 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.972 Theta(max)= 33.251

| | |
|--------------------------------|-------------------|
| R(reflections)= 0.0460(11225) | wR2(reflections)= |
| S = 0.861 | 0.1466(16301) |
| Npar= 515 | |

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 | 4.9 | Ratio |
| PLAT220_ALERT_2_C | NonSolvent | Resd 1 | N | Ueq(max)/Ueq(min) | Range | 4.7 | Ratio |
| PLAT241_ALERT_2_C | High | 'MainMol' | | Ueq as Compared to Neighbors of | | N1A | Check |
| PLAT906_ALERT_3_C | Large K Value in the Analysis of Variance | | | | | 2.080 | Check |
| PLAT910_ALERT_3_C | Missing # of FCF Reflection(s) Below Theta(Min). | | | | | 6 | Note |
| PLAT911_ALERT_3_C | Missing FCF Refl Between Thmin & STh/L= | 0.600 | | | | 2 | Report |
| PLAT971_ALERT_2_C | Check Calcd Resid. Dens. | 0.81Ang | From N2N | | | 1.61 | eA-3 |



Alert level G

| | | | | | | | |
|-------------------|--|--------------|-------|----------------|-------|-------|--------|
| PLAT004_ALERT_5_G | Polymeric Structure Found with Maximum Dimension | | | | | 2 | Info |
| PLAT154_ALERT_1_G | The s.u.'s on the Cell Angles are Equal ..(Note) | | | | | 0.001 | Degree |
| PLAT171_ALERT_4_G | The CIF-Embedded .res File Contains EADP Records | | | | | 1 | Report |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) | Ru1 | --N1N | . | | 7.4 | s.u. |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) | Ru2 | --Cl5 | . | | 6.0 | s.u. |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) | Ru2 | --Cl6 | . | | 6.8 | s.u. |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) | Ru2 | --Cl7 | . | | 5.5 | s.u. |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) | Ru2 | --N2N | . | | 5.6 | s.u. |
| PLAT300_ALERT_4_G | Atom Site Occupancy of Na2 | | | Constrained at | | 0.5 | Check |
| PLAT301_ALERT_3_G | Main Residue Disorder | (Resd 1) | | | | 1% | Note |
| PLAT431_ALERT_2_G | Short Inter HL..A Contact | Cl6 | ..02N | . | | 3.16 | Ang. |
| | | 1-x,-y,1-z = | | | | 2_656 | Check |
| PLAT720_ALERT_4_G | Number of Unusual/Non-Standard Labels | | | | | 6 | Note |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF ... | | | | | 25.80 | Deg. |
| | NA2 -O43 -NA2 | 2_655 | 1_555 | 1_555 | | # 189 | Check |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle(s) in CIF ... | | | | | 23.72 | Deg. |
| | NA2 -N1A -NA2 | 2_655 | 1_555 | 1_555 | | # 271 | Check |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= | 0.600 | | | | 460 | Note |
| PLAT933_ALERT_2_G | Number of HKL-OMIT Records in Embedded .res File | | | | | 4 | Note |
| PLAT941_ALERT_3_G | Average HKL Measurement Multiplicity | | | | | 2.7 | Low |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. | | | | | 2 | Info |

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

7 **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

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

12 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

6 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check

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.

