checkCIF/PLATON report

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

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: NZ1388_sqd

```
Bond precision:  C-C = 0.0242 A          Wavelength=0.71073

Cell:            a=18.915(4)     b=33.032(7)       c=36.635(7)
                 alpha=90        beta=95.62(3)     gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	22780(8)	22779(8)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	2(C200 H184 Ag6 N8 O12 P8 Re4), 4(F6 P), 10(C6 H6), C3 H3	?
Sum formula	C463 H431 Ag12 F24 N16 O24 P20 Re8	C231.50 H215.50 Ag6 F12 N8 O12 P10 Re4
Mr	10462.68	5231.33
Dx,g cm-3	1.525	1.525
Z	2	4
Mu (mm-1)	2.732	2.757
F000	10386.0	10386.0
F000’	10357.83	
h,k,lmax	24,43,48	24,42,48
Nref	54531	53736
Tmin,Tmax	0.754,0.896	0.754,1.000
Tmin’	0.478	

```
Correction method= # Reported T Limits: Tmin=0.754 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.985          Theta(max)= 27.918

R(reflections)= 0.1040( 44755)    wR2(reflections)= 0.2385( 53736)

S = 1.064                 Npar= 2562
```

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 A

```
PLAT331_ALERT_2_A Small Average Phenyl   C-C Dist. C270   -C275          1.33 Ang.
```

Author Response: These atoms are in a benzene solvate molecule that has high thermal displacement/some disorder.

Alert level B

```
DIFMN02_ALERT_2_B  The minimum difference density is < -0.1*ZMAX*1.00
           _refine_diff_density_min given =     -9.080
           Test value =     -7.500
DIFMX01_ALERT_2_B  The maximum difference density is > 0.1*ZMAX*1.00
           _refine_diff_density_max given =      8.926
           Test value =      7.500
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density       8.93 eA-3
PLAT098_ALERT_2_B Large Reported Min.  (Negative) Residual Density      -9.08 eA-3
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) .......          2 Report
PLAT213_ALERT_2_B Atom C54             has ADP max/min Ratio .....        4.3 prolat
PLAT213_ALERT_2_B Atom C219            has ADP max/min Ratio .....        4.3 prolat
PLAT220_ALERT_2_B Large Non-Solvent  C     Ueq(max)/Ueq(min) Range      10.0 Ratio
PLAT222_ALERT_3_B Large Non-Solvent  H     Uiso(max)/Uiso(min) ...       8.5 Ratio
PLAT241_ALERT_2_B High      Ueq as Compared to Neighbors for .....       C219 Check
PLAT242_ALERT_2_B Low       Ueq as Compared to Neighbors for .....       C131 Check
PLAT250_ALERT_2_B Large U3/U1 Ratio for Average U(i,j) Tensor ....        7.7 Note
PLAT331_ALERT_2_B Small Average Phenyl   C-C Dist. C297   -C302          1.35 Ang.
```

Author Response: These atoms are in a benzene solvate molecule that has high thermal displacement/some disorder.

```
PLAT331_ALERT_2_B Small Average Phenyl   C-C Dist. C303   -C305_a        1.35 Ang.
```

Author Response: These atoms are in a benzene solvate molecule that has high thermal displacement/some disorder.

```
PLAT332_ALERT_2_B Large Phenyl C-C Range           C288   -C293          0.26 Ang.
PLAT342_ALERT_3_B Low Bond Precision on  C-C Bonds ..............     0.0242 Ang.
```

Alert level C

```
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
           The relevant atom site should be identified.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
RFACG01_ALERT_3_C  The value of the R factor is > 0.10
           R factor given   0.104
PLAT213_ALERT_2_C Atom O140            has ADP max/min Ratio .....        3.7 prolat
PLAT213_ALERT_2_C Atom C134            has ADP max/min Ratio .....        3.3 prolat
PLAT213_ALERT_2_C Atom C218            has ADP max/min Ratio .....        3.2 prolat
PLAT214_ALERT_2_C Atom F261    (Anion/Solvent) ADP max/min Ratio          4.2 prolat
```

```
PLAT220_ALERT_2_C Large Non-Solvent  O     Ueq(max)/Ueq(min) Range        4.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C21    --  C22     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C105   --  C108    ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C120   --  C121    ..       0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C160   --  C161    ..       0.19 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C124 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C139 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C153 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C160 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C232 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....       N119 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C52 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C83 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....       C105 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....       C109 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....       C143 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....       C217 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....       C220 Check
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors of        C270 Check
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors of        C273 Check
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors of        C278 Check
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors of        C301 Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        C272 Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        C275 Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        C277 Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        C300 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.2 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.5 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        3.0 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.2 Note
PLAT373_ALERT_2_C Long   C(sp)-C(sp)   Bond  C12    -   C13    ...       1.37 Ang.
PLAT373_ALERT_2_C Long   C(sp)-C(sp)   Bond  C16    -   C17    ...       1.39 Ang.
PLAT373_ALERT_2_C Long   C(sp)-C(sp)   Bond  C20    -   C21    ...       1.40 Ang.
PLAT373_ALERT_2_C Long   C(sp)-C(sp)   Bond  C24    -   C25    ...       1.38 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H53C   ..  H161    ..       2.04 Ang.
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         34 Note
PLAT045_ALERT_1_G Calculated and Reported Z Differ by .............       0.50 Ratio
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      490.26 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          8 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records          3 Report
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of        P250 Check
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of        P260 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C288   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C289   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C290   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C291   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C292   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C293   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H288   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H289   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H290   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H291   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H292   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H293   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C312   is Constrained at      0.500 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of *C313   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C314   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H312   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H313   is Constrained at      0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H314   is Constrained at      0.500 Check
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =          9 Note
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for     C14    Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for     C18    Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for     C22    Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for     C26    Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C312   ..  C314    ..       1.36 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C312   ..  C313    ..       2.35 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C312   ..  C312    ..       2.76 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C313   ..  C314    ..       2.22 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C313   ..  C313    ..       2.59 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C314   ..  C314    ..       2.59 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         40 Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           ! Info
PLAT984_ALERT_1_G The Ag-f'=    -0.897 Deviates from the B&C-Value     -0.875 Check
PLAT984_ALERT_1_G The Re-f'=    -1.018 Deviates from the B&C-Value     -0.935 Check
PLAT985_ALERT_1_G The Re-f"=     7.231 Deviates from the B&C-Value      7.260 Check
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  1 ALERT level A = Most likely a serious problem - resolve or explain
 16 ALERT level B = A potentially serious problem, consider carefully
 43 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 43 ALERT level G = General information/check it is not something unexpected

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

PLATON version of 21/06/2015; check.def file version of 21/06/2015

Datablock NZ1388_sqd - ellipsoid plot