checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kv911

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: kv911

Bond precision: C-C = 0.0436 A   Wavelength=1.54178

Cell: a=23.7380(7)   b=20.5122(6)   c=29.8804(9)
               alpha=90   beta=93.370(2)   gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	14524.2(7)	14524.2(7)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C103 H104 Mn5 N17 O13 Re, C21 H27 Mn N2 O4, 2(F6 P), 3(C3 H7 O)	C103 H108 Mn5 N17 O13 Re, C21 H28 Mn N2 O4, 2(F6 P), 3(C3 H8 O)
Sum formula	C133 H152 F12 Mn6 N19 O20 P2 Re	C133 H160 F12 Mn6 N19 O20 P2 Re
Mr	3142.53	3150.51
Dx,g cm-3	1.437	1.437
Z	4	4
Mu (mm-1)	6.609	6.609
F000	6424.0	6424.0
F000'	6411.77	
h,k,lmax	19,17,25	19,17,25
Nref	8982	8642
Tmin,Tmax	0.374,0.424	0.414,0.748
Tmin'	0.283	

Correction method= # Reported T Limits: Tmin=0.414 Tmax=0.748
AbsCorr = MULTI-SCAN

Data completeness= 0.962   Theta(max)= 40.289

R(reflections)= 0.1082(5302)   wR2(reflections)= 0.2250(8642)

S = 1.075   Npar= 1053

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**

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
            Calculated sin(theta_max)/wavelength =   0.4194

> **Author Response: Relatively poor crystals could only be grown which give no detectable diffraction below resolution d of 1.2 Ang. All efforts to harvest the crystal of better quality as well as crystallization attempts were not successful. Thus the data were collected up to this resolution.**

PLAT201_ALERT_2_A Isotropic non-H Atoms in Main Residue(s) ....   97 Report

> **Author Response: Due to relatively low ratio of reflections to parameters light atoms were not refined anisotropically.**

🟠 **Alert level B**

PLAT220_ALERT_2_B Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range   10.0 Ratio

> **Author Response: Most likely this is due to slight disorder of coordinated water and/or i-propanole molecules which was not resolved as not to complicate the model.**

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ....   0.0436 Ang.

> **Author Response: This is due to relatively low quality of the data.**

PLAT420_ALERT_2_B D-H Without Acceptor   O00L   -- H00A   ...   Please Check

> **Author Response: O00L is assigned to coordinated water molecule; the first of its H ato takes part in D-H hydrogen bond formation, while the second (H00A) does not and, in principle, can be disordered.**

PLAT430_ALERT_2_B Short Inter D...A Contact O1   .. O1AA   ..   2.66 Ang.

> **Author Response: These distances are slightly shorter than expected for H-bonding due to disorder of solvent molecules: O1 and O4AA atoms have refined Uiso of ca. 0.25.Thus their relative positions can be slightly different comparing to the proposed model.**

PLAT430_ALERT_2_B Short Inter D...A Contact O1   .. O02Z   ..   2.75 Ang.

Author Response: These distances are slightly shorter than expected for H-bonding due to disorder of solvent molecules: O1 and O4AA atoms have refined Uiso of ca. 0.25.Thus their relative positions can be slightly different comparing to the proposed model.

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PLAT430_ALERT_2_B Short Inter D...A Contact  O4AA   ..  N017    ..       2.80 Ang.
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Author Response: These distances are slightly shorter than expected for H-bonding due to disorder of solvent molecules: O1 and O4AA atoms have refined Uiso of ca. 0.25.Thus their relative positions can be slightly different comparing to the proposed model.

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🟡 **Alert level C**

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REFNR01_ALERT_3_C  Ratio of reflections to parameters is < 10 for a
            centrosymmetric structure
            sine(theta)/lambda              0.4194
            Proportion of unique data used  1.0000
            Ratio reflections to parameters 8.2070
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .    0.962 Note
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ   Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..    7.98 Check
PLAT082_ALERT_2_C High R1 Value ...............................    0.11 Report
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ...................    8.21 Note
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........     45 Check
PLAT213_ALERT_2_C Atom N00X           has ADP max/min Ratio .....    3.2 prolat
PLAT222_ALERT_3_C Non-Solvent Resd 1   H Uiso(max)/Uiso(min) Range    5.9 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   N00X Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   N01L Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C02X Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C03H Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C03K Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C04C Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C033 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C040 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C044 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C047 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   O013 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C04D Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   Mn05 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   Mn07 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   N00U Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   N00Y Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C00Z Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C01C Check
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   C01H Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C01J Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    C12 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C02B Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C02R Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C03C Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C03E Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C03I Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C03Q Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C04M Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C036 Check
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PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of      C042 Check
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of      C03J Check
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of      C03V Check
PLAT243_ALERT_4_C High    'Solvent' Ueq as Compared to Neighbors of      C6AA Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........        O1 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........      O1AA Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........      O4AA Check
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond   C7     -   C11    ..     1.36 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond   C03S   -   C04C   ..     1.41 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn      H15C   ..  H3AA   ..     1.87 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn      H8C    ..  H10C   ..     2.05 Ang.
PLAT430_ALERT_2_C Short Inter D...A Contact   O00H   ..  O013   ..     2.85 Ang.
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Author Response: These distances are slightly shorter than expected for H-bonding due to disorder of solvent molecules: O1 and O4AA atoms have refined Uiso of ca. 0.25. Thus their relative positions can be slightly different comparing to the proposed model.

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PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .        32 Ang3
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......    20.504 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     3.947 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     2.404 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.419       339 Report
PLAT975_ALERT_2_C Check Calcd Residual Density  0.85A From     O02Z     0.54 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density  0.82A From     O02Z     0.47 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.         0 Note
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⬤ **Alert level G**

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
          _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C133 H160 F12 Mn6 N19 O20 P2 R
            Atom count from the _atom_site data:  C133 H152 F12 Mn6 N19 O20 P2 R
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z     4
          From the CIF: _chemical_formula_sum  C133 H160 F12 Mn6 N19 O20 P2 Re
          TEST: Compare cell contents of formula and atom_site data

          atom     Z*formula  cif sites diff
          C         532.00    532.00    0.00
          H         640.00    608.00   32.00
          F          48.00     48.00    0.00
          Mn         24.00     24.00    0.00
          N          76.00     76.00    0.00
          O          80.00     80.00    0.00
          P           8.00      8.00    0.00
          Re          4.00      4.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          15 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          9 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ   Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large   506.60 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          7 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT244_ALERT_4_G Low     'Solvent' Ueq as Compared to Neighbors of     P008 Check
PLAT244_ALERT_4_G Low     'Solvent' Ueq as Compared to Neighbors of     P009 Check
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PLAT343_ALERT_2_G Unusual sp3       Angle Range in Main Residue for     C05G Check
PLAT344_ALERT_2_G Unusual      sp3 Angle Range in Solvent/Ion for .     C0AA Check
PLAT344_ALERT_2_G Unusual      sp? Angle Range in Solvent/Ion for .     C3AA Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C3AA    -    C5AA   ..     1.52 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........      306 Note
PLAT721_ALERT_1_G Bond    Calc    0.97000, Rep    0.96000 Dev...       0.01 Ang.
                  C2AA   -H2AB        1.555   1.555 ............     #  344 Check
PLAT721_ALERT_1_G Bond    Calc    0.97000, Rep    0.96000 Dev...       0.01 Ang.
                  C8     -H8A         1.555   1.555 ............     #  346 Check
PLAT721_ALERT_1_G Bond    Calc    0.97000, Rep    0.96000 Dev...       0.01 Ang.
                  C8     -H8B         1.555   1.555 ............     #  347 Check
PLAT721_ALERT_1_G Bond    Calc    0.97000, Rep    0.96000 Dev...       0.01 Ang.
                  C15    -H15C        1.555   1.555 ............     #  358 Check
PLAT722_ALERT_1_G Angle   Calc     108.00, Rep     109.50 Dev...       1.50 Degree
                  H8A    -C8     -H8B        1.555   1.555   1.555  #  663 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        6 Note
                  C3 H7 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        7 Note
                  C3 H7 O
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters       1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       72 Note
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) Still        47 % Note
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   2 ALERT level A = Most likely a serious problem - resolve or explain
   6 ALERT level B = A potentially serious problem, consider carefully
  59 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  29 ALERT level G = General information/check it is not something unexpected

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

PLATON version of 27/03/2017; check.def file version of 24/03/2017

NOMOVE FORCED

Prob = 50
Temp = 298

-1 Y

PLATON-Aug 3 09:30:03 2017 - (70316)

Z 1   kv911   P 1 21/n 1   R = 0.11   RES=   0   -6 X