checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kv883

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: kv883

Bond precision: C-C = 0.0063 A   Wavelength=0.71073

Cell: a=14.2002(9)   b=15.7993(9)   c=18.0470(11)
               alpha=84.638(3)   beta=82.694(4)   gamma=65.057(3)
Temperature: 200 K

	Calculated	Reported
Volume	3637.9(4)	3637.9(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C18 H22 Mn N2 O6), C24 H20 P, C7 N7 Re, 6(O)	C7 N7 Re, 2(C18 H22 Mn N2 O6), C24 H20 P, 6(O)
Sum formula	C67 H64 Mn2 N11 O18 P Re	C67 H64 Mn2 N11 O18 P Re
Mr	1638.35	1638.34
Dx,g cm-3	1.496	1.496
Z	2	2
Mu (mm-1)	2.098	2.098
F000	1654.0	1654.0
F000'	1654.19	
h,k,lmax	19,21,24	19,21,24
Nref	19133	18851
Tmin,Tmax	0.692,0.761	0.553,0.746
Tmin'	0.528	

Correction method= # Reported T Limits: Tmin=0.553 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.985   Theta(max)= 28.881

R(reflections)= 0.0394(16297)   wR2(reflections)= 0.0978(18851)

S = 1.120   Npar= 909

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 B

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ....   O1S Check

Author Response: These oxygen atoms are those of solvent water molecules. Hydrogen atoms were not localized because of their disorder. For instance, the distances between equivalent pairs O1S - O1S' and O4S - O4S' are short enough (of ca. 2.85 Ang.) to reveal hydrogen bond; however, due to the presence of inversion center, it is not possible to place H atom with full occupancy between these oxygens.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ....   O2S Check

Author Response: These oxygen atoms are those of solvent water molecules. Hydrogen atoms were not localized because of their disorder. For instance, the distances between equivalent pairs O1S - O1S' and O4S - O4S' are short enough (of ca. 2.85 Ang.) to reveal hydrogen bond; however, due to the presence of inversion center, it is not possible to place H atom with full occupancy between these oxygens.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ....   O3S Check

Author Response: These oxygen atoms are those of solvent water molecules. Hydrogen atoms were not localized because of their disorder. For instance, the distances between equivalent pairs O1S - O1S' and O4S - O4S' are short enough (of ca. 2.85 Ang.) to reveal hydrogen bond; however, due to the presence of inversion center, it is not possible to place H atom with full occupancy between these oxygens.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ....   O4S Check

Author Response: These oxygen atoms are those of solvent water molecules. Hydrogen atoms were not localized because of their disorder. For instance, the distances between equivalent pairs O1S - O1S' and O4S - O4S' are short enough (of ca. 2.85 Ang.) to reveal hydrogen bond; however, due to the presence of inversion center, it is not possible to place H atom with full occupancy between these oxygens.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ....   O5S Check

Author Response: These oxygen atoms are those of solvent water molecules. Hydrogen atoms were not localized because of their disorder. For instance, the distances between equivalent pairs O1S - O1S' and O4S - O4S' are short enough (of ca. 2.85 Ang.) to reveal hydrogen bond; however, due to the presence of inversion center, it is not possible to place H atom with full occupancy between these oxygens.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ....   O6S Check

Author Response: These oxygen atoms are those of solvent water molecules. Hydrogen atoms were not localized because of their disorder. For instance, the distances between equivalent pairs O1S - O1S' and O4S - O4S' are short enough (of ca. 2.85 Ang.) to reveal hydrogen bond; however, due to the presence of inversion center, it is not possible to place H atom with full occupancy between these oxygens.

PLAT430_ALERT_2_B Short Inter D...A Contact O1S   .. O2S   ..   2.81 Ang.

Author Response: These oxygen atoms are those of solvent water molecules. Hydrogen atoms were not localized because of their disorder. For instance, the distances between equivalent pairs O1S - O1S' and O4S - O4S' are short enough (of ca. 2.85 Ang.) to reveal hydrogen bond; however, due to the presence of inversion center, it is not possible to place H atom with full occupancy between these oxygens.

PLAT430_ALERT_2_B Short Inter D...A Contact O1S   .. O1S   ..   2.82 Ang.

Author Response: These oxygen atoms are those of solvent water molecules. Hydrogen atoms were not localized because of their disorder. For instance, the distances between equivalent pairs O1S - O1S' and O4S - O4S' are short enough (of ca. 2.85 Ang.) to reveal hydrogen bond; however, due to the presence of inversion center, it is not possible to place H atom with full occupancy between these oxygens.

PLAT430_ALERT_2_B Short Inter D...A Contact O1S   .. O6S   ..   2.83 Ang.

Author Response: These oxygen atoms are those of solvent water molecules. Hydrogen atoms were not localized because of their disorder. For instance, the distances between equivalent pairs O1S - O1S' and O4S - O4S' are short enough (of ca. 2.85 Ang.) to reveal hydrogen bond; however, due to the presence of inversion center, it is not possible to place H atom with full occupancy between these oxygens.

PLAT430_ALERT_2_B Short Inter D...A Contact O2S   .. N35   ..   2.86 Ang.

Author Response: These oxygen atoms are those of solvent water molecules. Hydrogen atoms were not localized because of their disorder. For instance, the distances between equivalent pairs O1S - O1S' and O4S - O4S' are short enough (of ca. 2.85 Ang.) to reveal hydrogen bond; however, due to the presence of inversion center, it is not possible to place H atom with full occupancy between these oxygens.

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PLAT430_ALERT_2_B Short Inter D...A Contact  O3S    .. O6S     ..     2.79 Ang.
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Author Response: These oxygen atoms are those of solvent water molecules. Hydrogen atoms were not localized because of their disorder. For instance, the distances between equivalent pairs O1S - O1S' and O4S - O4S' are short enough (of ca. 2.85 Ang.) to reveal hydrogen bond; however, due to the presence of inversion center, it is not possible to place H atom with full occupancy between these oxygens.

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PLAT430_ALERT_2_B Short Inter D...A Contact  O3S    .. N34     ..     2.85 Ang.
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Author Response: These oxygen atoms are those of solvent water molecules. Hydrogen atoms were not localized because of their disorder. For instance, the distances between equivalent pairs O1S - O1S' and O4S - O4S' are short enough (of ca. 2.85 Ang.) to reveal hydrogen bond; however, due to the presence of inversion center, it is not possible to place H atom with full occupancy between these oxygens.

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PLAT430_ALERT_2_B Short Inter D...A Contact  O4S    .. O5S     ..     2.80 Ang.
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Author Response: These oxygen atoms are those of solvent water molecules. Hydrogen atoms were not localized because of their disorder. For instance, the distances between equivalent pairs O1S - O1S' and O4S - O4S' are short enough (of ca. 2.85 Ang.) to reveal hydrogen bond; however, due to the presence of inversion center, it is not possible to place H atom with full occupancy between these oxygens.

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PLAT430_ALERT_2_B Short Inter D...A Contact  O4S    .. O6S     ..     2.82 Ang.
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Author Response: These oxygen atoms are those of solvent water molecules. Hydrogen atoms were not localized because of their disorder. For instance, the distances between equivalent pairs O1S - O1S' and O4S - O4S' are short enough (of ca. 2.85 Ang.) to reveal hydrogen bond; however, due to the presence of inversion center, it is not possible to place H atom with full occupancy between these oxygens.

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PLAT430_ALERT_2_B Short Inter D...A Contact  O4S    .. O4S     ..     2.84 Ang.
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Author Response: These oxygen atoms are those of solvent water molecules. Hydrogen atoms were not localized because of their disorder. For instance, the distances between equivalent pairs O1S - O1S' and O4S - O4S' are short enough (of ca. 2.85 Ang.) to reveal hydrogen bond; however, due to the presence of inversion center, it is not possible to place H atom with full occupancy between these oxygens.

🟡 **Alert level C**
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PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....      2.78 Report
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C45 Check
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .        44 Ang3
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #         1 Note
              C18 H22 Mn N2 O6
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     2.009 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600         68 Report
PLAT971_ALERT_2_C Check Calcd Residual Density  2.16A From     C114      1.98 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density  0.84A From     Re1       1.85 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density  0.84A From     Re1       1.70 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density  0.93A From     O2S       0.79 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density  1.07A From     O6S       0.64 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density  0.41A From     O6S      -0.49 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density  0.51A From     O6S      -0.43 eA-3
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⚪ **Alert level G**
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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         8 Report
PLAT012_ALERT_1_G No     _shelx_res_checksum found in CIF ........  Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ  Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      7.99 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Re1     -- C37     ..       5.2 s.u.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         2 Note
              C18 H22 Mn N2 O6
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         5 Note
              O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         6 Note
              O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         7 Note
              O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        10 Note
              O
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)          2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        212 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          7 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
  15 ALERT level B = A potentially serious problem, consider carefully
  13 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  29 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   7 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.

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