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: test

```
Bond precision:  C-C = 0.0075 A          Wavelength=0.71073

Cell:           a=22.3274(18)    b=14.7217(12)     c=23.2155(18)
                alpha=90         beta=98.282(1)    gamma=90
Temperature:    293 K
```

	Calculated	Reported
Volume	7551.3(10)	7551.3(10)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	2(C33 H30 Cr Mn N8 O5), 2(C H4 O), 5(H2 O)	2(C33 H30 Cr Mn N8 O5), 2(C H4 O), 5(H2 O)
Sum formula	C68 H78 Cr2 Mn2 N16 O17	C34 H39 Cr Mn N8 O8.50
Mr	1605.34	802.67
Dx,g cm-3	1.412	1.412
Z	4	8
Mu (mm-1)	0.683	0.683
F000	3328.0	3328.0
F000’	3334.56	
h,k,lmax	26,17,27	26,17,27
Nref	6654	6617
Tmin,Tmax	0.809,0.855	0.816,0.859
Tmin’	0.809	

```
Correction method= MULTI-SCAN

Data completeness= 0.994          Theta(max)= 25.000

R(reflections)= 0.0534( 4643)     wR2(reflections)= 0.1679( 6617)

S = 1.095                 Npar= 477
```

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

PLAT417_ALERT_2_A Short Inter D-H..H-D H6B .. H8A .. 1.44 Ang.

Author Response: The electron density arround the solvent O atoms is somewhat weak, \ therefore making it difficult accurately confirm the right position of the H atoms bonded to the O atom.

PLAT417_ALERT_2_A Short Inter D-H..H-D H7A .. H9A .. 1.70 Ang.

Author Response: The electron density arround the solvent O atoms is somewhat weak, \ therefore making it difficult accurately confirm the right position of the H atoms bonded to the O atom.

PLAT417_ALERT_2_A Short Inter D-H..H-D H7B .. H9A .. 1.76 Ang.

Author Response: The electron density arround the solvent O atoms is somewhat weak, \ therefore making it difficult accurately confirm the right position of the H atoms bonded to the O atom.

Alert level B

PLAT241_ALERT_2_B High Ueq as Compared to Neighbors for ..... C33 Check
PLAT417_ALERT_2_B Short Inter D-H..H-D H6A .. H8A .. 2.04 Ang.

Author Response: The electron density arround the solvent O atoms is somewhat weak, \ therefore making it difficult accurately confirm the right position of the H atoms bonded to the O atom.

PLAT417_ALERT_2_B Short Inter D-H..H-D H7A .. H7A .. 1.80 Ang.

Author Response: The electron density arround the solvent O atoms is somewhat weak, \ therefore making it difficult accurately confirm the right position of the H atoms bonded to the O atom.

PLAT417_ALERT_2_B Short Inter D-H..H-D H7A .. H7B .. 2.05 Ang.

Author Response: The electron density arround the solvent O atoms is somewhat weak, \ therefore making it difficult accurately confirm the right position of the H atoms bonded to the O atom.

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PLAT420_ALERT_2_B D-H Without Acceptor       O7     -   H7B    ...     Please Check
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Alert level C

```
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        3.6 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C31    --  C32     ..       0.19 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C19 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C32 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....         N7 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0075 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C31    -   C32    ...       1.40 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C32    -   C33    ...       1.36 Ang.
PLAT417_ALERT_2_C Short Inter D-H..H-D       H7A    ..  H9A     ..       2.14 Ang.
```

Author Response: The electron density arround the solvent O atoms is somewhat weak, \ therefore making it difficult accurately confirm the right position of the H atoms bonded to the O atom.

Alert level G

```
FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C34 H39 Cr1 Mn1 N8 O8.5
           Atom count from _chemical_formula_moiety:C68 H78 Cr2 Mn2 N16 O17
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          8 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ............       0.50 Ratio
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
```

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

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  15 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   1 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*, 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 24/07/2014; check.def file version of 24/07/2014

Datablock test - ellipsoid plot