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: dp

Bond precision: C-C = 0.0156 A Wavelength=0.71073

Cell: a=15.216(10) b=15.491(10) c=17.603(14)
alpha=90 beta=93.895(11) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	4140(5)	4140(5)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	?
Moiety formula	C34 H32 Cr Mn N8 O5, C H4 O, 3(H2 O)	C34 H32 Cr Mn N8 O5, C H4 O, 3(H2 O)
Sum formula	C35 H42 Cr Mn N8 O9	C35 H42 Cr Mn N8 O9
Mr	825.71	825.71
Dx,g cm-3	1.325	1.325
Z	4	4
Mu (mm-1)	0.626	0.626
F000	1716.0	1716.0
F000’	1719.31	
h,k,lmax	18,18,20	16,18,19
Nref	7287	7117
Tmin,Tmax	0.914,0.933	0.912,0.934
Tmin’	0.910	

Correction method= MULTI-SCAN

Data completeness= 0.977 Theta(max)= 25.000

R(reflections)= 0.0826(4690) wR2(reflections)= 0.2438(7117)

S = 1.009 Npar= 490

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

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PLAT213_ALERT_2_B Atom C23             has ADP max/min Ratio .....        4.1 prolat
PLAT220_ALERT_2_B Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        7.8 Ratio
PLAT222_ALERT_3_B Large Non-Solvent    H    Uiso(max)/Uiso(min) ..        7.6 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C28    --  C29     ..        8.1 su
PLAT242_ALERT_2_B Low       Ueq as Compared to Neighbors for .....       C22 Check
PLAT341_ALERT_3_B Low Bond Precision on  C-C Bonds ..............    0.0156 Ang.
PLAT360_ALERT_2_B Short  C(sp3)-C(sp3) Bond  C22    -   C23    ...      1.25 Ang.
PLAT410_ALERT_2_B Short Intra H...H Contact  H18    ..  H22A   ..      1.85 Ang.
PLAT420_ALERT_2_B D-H Without Acceptor       O6     -   H6A    ...    Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O7     -   H7A    ...    Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O9     -   H9A    ...    Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O9     -   H9B    ...    Please Check
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Alert level C

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PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......     0.977 Note
PLAT213_ALERT_2_C Atom C22             has ADP max/min Ratio .....        3.6 prolat
PLAT234_ALERT_4_C Large Hirshfeld Difference O4     --  C17     ..      0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N3     --  C3      ..      0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N5     --  C9      ..      0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C7     --  C8      ..      0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C10    --  C11     ..      0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C15    --  C21     ..      0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C25    --  C26     ..      0.16 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        N1 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C6 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C8 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C28 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        O4 Check
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H22A   ..  H23B    ..      1.89 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H22B   ..  H23A    ..      1.88 Ang.
PLAT417_ALERT_2_C Short Inter D-H..H-D       H7B    ..  H9A     ..      2.12 Ang.
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Alert level G

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PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF    Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         9 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical        ? Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.      0.12 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)       293 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        39 Check
             H6B  -O6   -H6B     1.555   1.555   1.555             0.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        42 Check
             H7B  -O7   -H7B     1.555   1.555   1.555             0.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        45 Check
             H7A  -O7   -H7A     1.555   1.555   1.555             0.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        50 Check
             H9B  -O9   -H9B     1.555   1.555   1.555             0.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        51 Check
             H9A  -O9   -H9A     1.555   1.555   1.555             0.00 Deg.
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL      2014 Note
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           2 Units
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
12 **ALERT level B** = A potentially serious problem, consider carefully
17 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected

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  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 20 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
 13 ALERT type 4 Improvement, methodology, query or suggestion
  3 ALERT type 5 Informative message, check
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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 20/08/2014; check.def file version of 18/08/2014

Datablock dp - ellipsoid plot