checkCIF (full publication check) running

checkCIF/PLATON (full publication check)

Structure factors have been supplied for datablock(s) I

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
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: I

```
Bond precision:        C-C = 0.0050 A                  Wavelength=0.71073
Cell:         a=5.2482(9)       b=6.5330(11)      c=10.6128(18)
              alpha=90.532(10)  beta=102.774(11)  gamma=109.139(10)
Temperature: 150 K
                     Calculated                          Reported
Volume               333.93(10)                          333.93(10)
Space group          P -1                                P -1
Hall group           -P 1                                -P 1
Moiety formula       C6 H10 Mn N8 O6, 2(H2 O)            C6 H10 Mn N8 O6, 2(H2 O)
Sum formula          C6 H14 Mn N8 O8                     C6 H14 Mn N8 O8
Mr                   381.19                              381.19
Dx,g cm-3            1.896                               1.896
Z                    1                                   1
Mu (mm-1)            1.052                               1.052
F000                 195.0                               195.0
F000'                195.43
h,k,lmax             6,8,13                              6,8,13
Nref                 1530                                1519
Tmin,Tmax            0.951,0.969                         0.951,0.971
Tmin'                0.919
Correction method= # Reported T Limits: Tmin=0.951 Tmax=0.971
AbsCorr = MULTI-SCAN
Data completeness= 0.993           Theta(max)= 27.482
R(reflections)= 0.0514( 1372)         wR2(reflections)= 0.0857( 1519)
S = 1.226               Npar= 131
```

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

PLAT417_ALERT_2_B Short Inter D-H..H-D H2WA .. H12A .. 1.94 Ang.

Author Response: Several reasons may explain this low value: i) the Hydrogen atoms are not pointing directly to each other; ii) atom H12A has an occupancy of only 25%, and when present the water molecule may accomodate its H-atoms in order to enlarge the H...H distance. However, the electron density distribution did not allow us the creation of a model of disorder for the water molecule; iii) only H...H distances of lower than 1.8 A are likely to not belivable. Additionally, any efforts to enlarge this distance (e.g. with DFIX) avoided sensible solutions.

Alert level C

PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 4.998 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 5 Report

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 7 Note
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 10 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Mn1 -- N14 .. 5.1 su
PLAT300_ALERT_4_G Atom Site Occupancy of >H11A is Constrained at 0.750 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <H12A is Constrained at 0.250 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 4 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 5 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ... 3 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 3 Note

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
5 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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checkCIF publication errors

Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
_publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
_publ_contact_author_phone are all missing.
At least one of these should be present.
PUBL006_ALERT_1_A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or
empty.

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7 **ALERT level A** = Data missing that is essential or data in wrong format
1 **ALERT level G** = General alerts. Data that may be required is missing

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Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

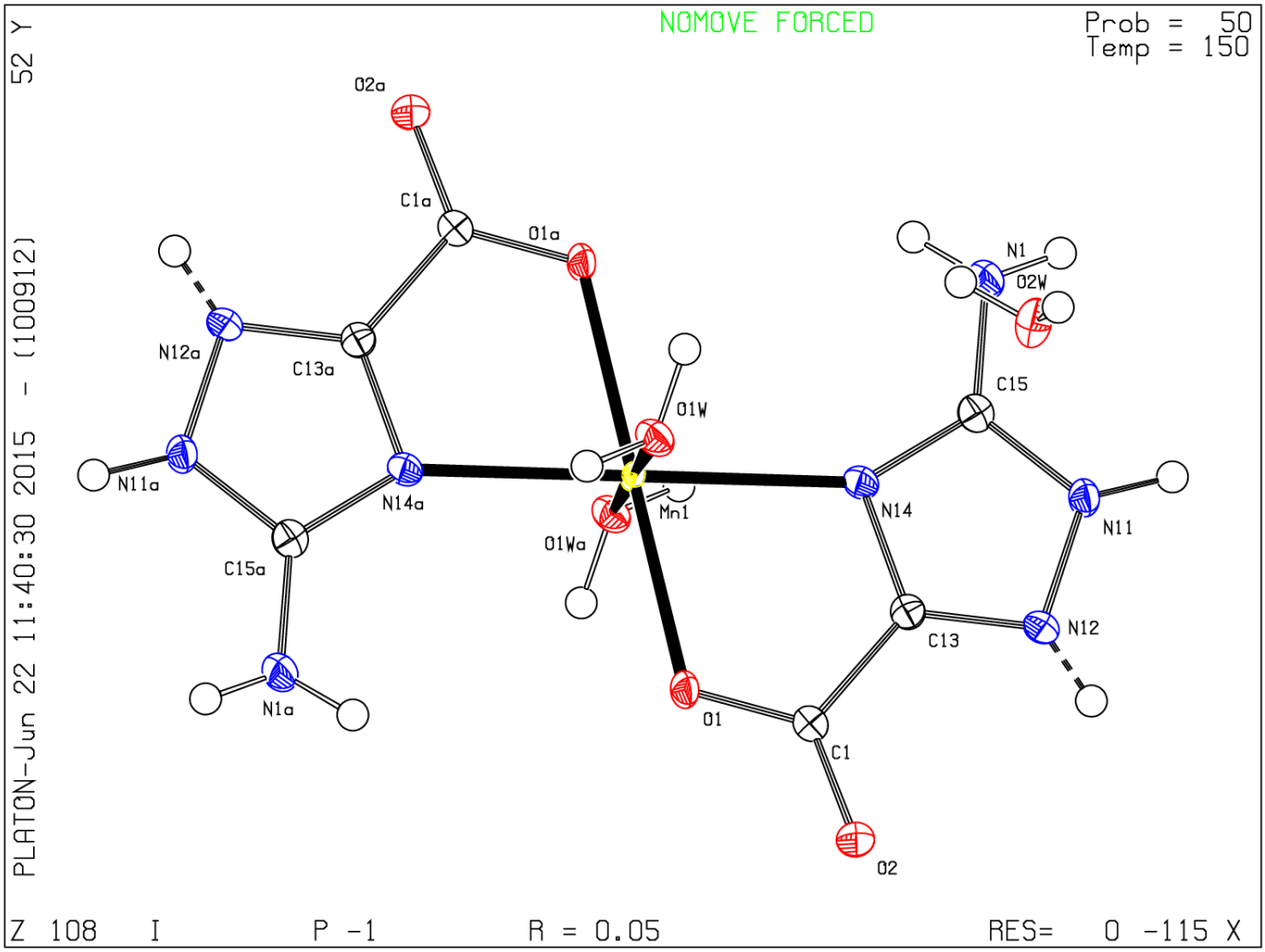
```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
```

;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
end Validation Reply Form

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

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

Datablock I - ellipsoid plot



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Test a new CIF entry