

checkCIF (basic structural check) running

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) hd141

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.
Please wait while processing

[CIF dictionary](#)
[Interpreting this report](#)

Datablock: hd141

Bond precision: N- N = 0.0080 Å Wavelength=0.71073

Cell: a=8.34800 b=10.15400 c=10.82300
alpha=68.3500 beta=71.5900 gamma=78.5500

Temperature: 293 K

	Calculated	Reported
Volume	805.553	806
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	Mo8 O26, 2(C2 H6 N4), 4(H2 O)	C4 H20 Mo8 N8 O30
Sum formula	C4 H20 Mo8 N8 O30	C4 H20 Mo8 N8 O30
Mr	1427.80	1427.80
Dx, g cm ⁻³	2.943	2.943
Z	1	1
Mu (mm ⁻¹)	3.127	3.127
F000	676.0	676.0
F000'	662.52	
h,k,lmax	10,12,13	10,12,13
Nref	3293	3277
Tmin,Tmax	0.739,0.731	0.272,0.535
Tmin'	0.724	

Correction method= # Reported T Limits: Tmin=0.272 Tmax=0.535 AbsCorr = PSI-SCAN

Data completeness= 0.995

Theta(max)= 26.370

R(reflections)= 0.0302(2807)

wR2(reflections)= 0.0915(3277)

S = 1.093

Npar= 227

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 C

PLAT141_ALERT_4_C s.u. on a - Axis Small or Missing 0.00000 Ang.
 PLAT142_ALERT_4_C s.u. on b - Axis Small or Missing 0.00000 Ang.
 PLAT143_ALERT_4_C s.u. on c - Axis Small or Missing 0.00000 Ang.
 PLAT144_ALERT_4_C s.u. on alpha Small or Missing 0.0000 Degree
 PLAT145_ALERT_4_C s.u. on beta Small or Missing 0.0000 Degree
 PLAT146_ALERT_4_C s.u. on gamma Small or Missing 0.0000 Degree
 PLAT151_ALERT_1_C No s.u. (esd) Given on Volume Please Do !
 PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) Ow2 - H7 .. 1.07 Ang.
 PLAT420_ALERT_2_C D-H Without Acceptor N3 -- H3A ... Please Check
 PLAT420_ALERT_2_C D-H Without Acceptor N3 -- H3B ... Please Check
 PLAT751_ALERT_4_C Bond Calc 1.00000, Rep 1.001(5) Senseless s.u.
 N1 -H1 1.555 1.555 Bond # 33 Check
 PLAT751_ALERT_4_C Bond Calc 0.77000, Rep 0.771(4) Senseless s.u.
 N2 -H2 1.555 1.555 Bond # 35 Check
 PLAT751_ALERT_4_C Bond Calc 0.89000, Rep 0.887(4) Senseless s.u.
 N4 -H4 1.555 1.555 Bond # 41 Check
 PLAT751_ALERT_4_C Bond Calc 0.97000, Rep 0.971(5) Senseless s.u.
 C1 -H5 1.555 1.555 Bond # 42 Check

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PLAT751_ALERT_4_C Bond Calc 0.98000, Rep 0.980(4) ..... Senseless s.u.
OW1 -H8 1.555 1.555 ..... Bond # 43 Check
PLAT751_ALERT_4_C Bond Calc 0.87000, Rep 0.871(4) ..... Senseless s.u.
OW1 -H9 1.555 1.555 ..... Bond # 44 Check
PLAT751_ALERT_4_C Bond Calc 0.97000, Rep 0.968(5) ..... Senseless s.u.
OW2 -H6 1.555 1.555 ..... Bond # 45 Check
PLAT751_ALERT_4_C Bond Calc 1.07000, Rep 1.074(5) ..... Senseless s.u.
OW2 -H7 1.555 1.555 ..... Bond # 46 Check
PLAT752_ALERT_4_C Angle Calc 139.00, Rep 139.2(6) ..... Senseless s.u.
C1 -N1 -H1 1.555 1.555 1.555 # 93
PLAT752_ALERT_4_C Angle Calc 113.00, Rep 113.0(5) ..... Senseless s.u.
N2 -N1 -H1 1.555 1.555 1.555 # 94
PLAT752_ALERT_4_C Angle Calc 109.00, Rep 109.2(5) ..... Senseless s.u.
C2 -N2 -H2 1.555 1.555 1.555 # 96
PLAT752_ALERT_4_C Angle Calc 142.00, Rep 141.6(5) ..... Senseless s.u.
N1 -N2 -H2 1.555 1.555 1.555 # 97
PLAT752_ALERT_4_C Angle Calc 118.00, Rep 118.2(5) ..... Senseless s.u.
C2 -N4 -H4 1.555 1.555 1.555 # 102
PLAT752_ALERT_4_C Angle Calc 132.00, Rep 132.0(5) ..... Senseless s.u.
C1 -N4 -H4 1.555 1.555 1.555 # 103
PLAT752_ALERT_4_C Angle Calc 127.00, Rep 126.8(6) ..... Senseless s.u.
N1 -C1 -H5 1.555 1.555 1.555 # 105
PLAT752_ALERT_4_C Angle Calc 125.00, Rep 124.8(5) ..... Senseless s.u.
N4 -C1 -H5 1.555 1.555 1.555 # 106
PLAT752_ALERT_4_C Angle Calc 122.00, Rep 121.6(5) ..... Senseless s.u.
H8 -OW1 -H9 1.555 1.555 1.555 # 110
PLAT752_ALERT_4_C Angle Calc 119.00, Rep 118.5(4) ..... Senseless s.u.
H6 -OW2 -H7 1.555 1.555 1.555 # 111

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Alert level G

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PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 9 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0. Degree
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _difrn_ambient_temperature ..... (K) 293 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 2 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.20 Ratio
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
28 **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

- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
27 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

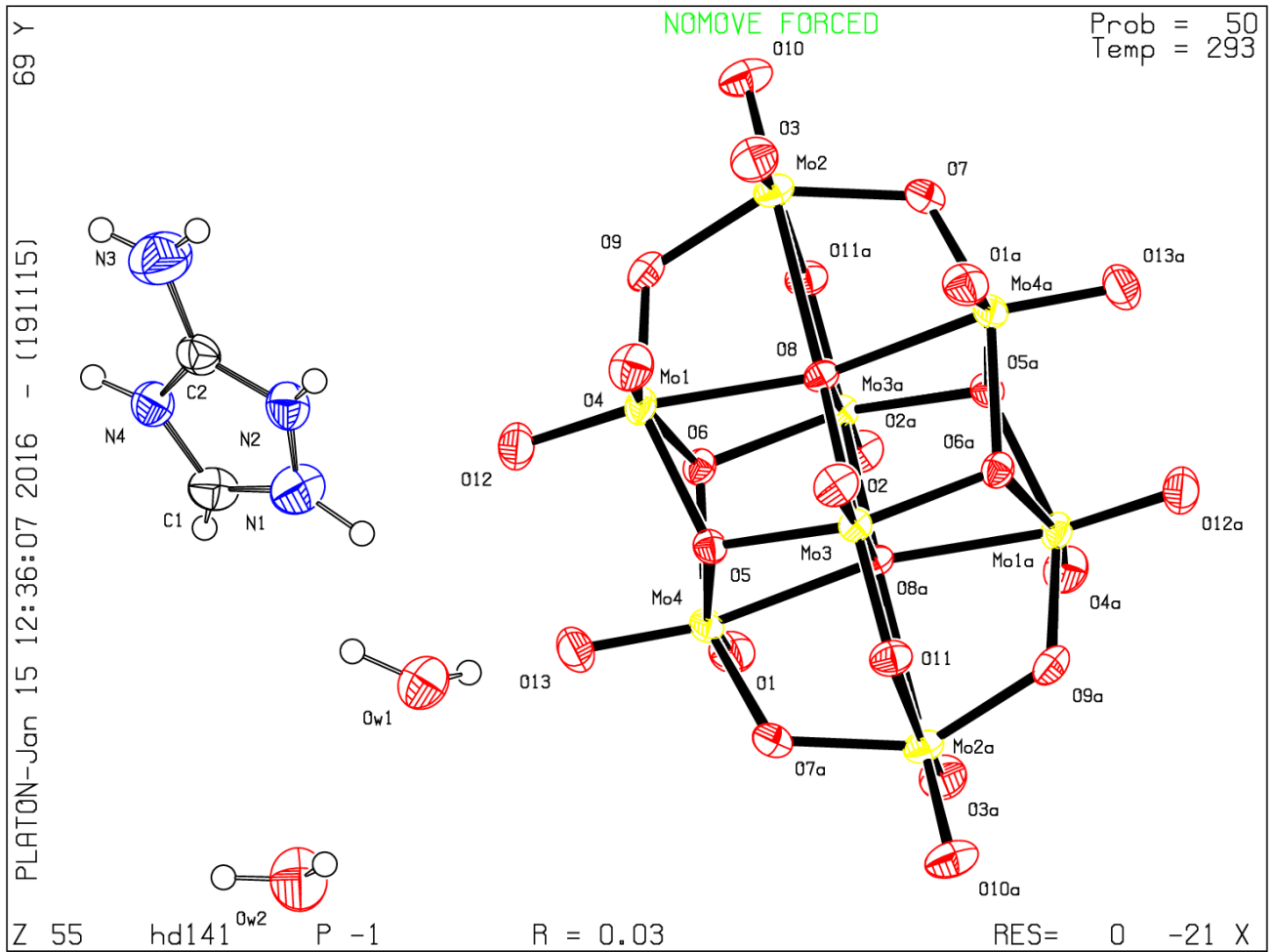
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 19/11/2015; check.def file version of 17/11/2015

Datablock hd141 - ellipsoid plot

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