

# 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: compound2

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Bond precision:    C-C = 0.0329 Å                      Wavelength=1.54184

Cell:                      a=19.0906(14)              b=8.5500(4)              c=17.2528(11)  
                            alpha=90                      beta=100.240(6)              gamma=90  
Temperature:              154 K

	Calculated	Reported
Volume	2771.2(3)	2771.2(3)
Space group	P 21/c	P 21/c
Hall group	: -P 2ybc	-P 2ybc
Moiety formula	C22 H19 Mn Mo N O5 P, C7 H8	C22 H19 Mn Mo N O5 P, C7 H8
Sum formula	C29 H27 Mn Mo N O5 P	C29 H27 Mn Mo N O5 P
Mr	651.37	651.37
Dx,g cm-3	1.561	1.561
Z	4	4
Mu (mm-1)	8.285	8.285
F000	1320.0	1360.0
F000'	1321.99	
h,k,lmax	23,10,20	22,10,20
Nref	5209	5094
Tmin,Tmax	0.429,0.661	0.491,1.000
Tmin'	0.197	

Correction method= # Reported T Limits: Tmin=0.491 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.978                      Theta(max)= 69.406

R(reflections)= 0.2410( 4275)              wR2(reflections)= 0.5492( 5094)

S = 2.389                      Npar= 305

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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

PLAT082_ALERT_2_A High R1 Value .....	0.24 Report
PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) .....	0.55 Report
PLAT097_ALERT_2_A Large Reported Max. (Positive) Residual Density	10.95 eA-3
PLAT213_ALERT_2_A Atom C7 has ADP max/min Ratio .....	5.1 prolat
PLAT213_ALERT_2_A Atom C10 has ADP max/min Ratio .....	6.7 prolat

### Alert level B

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) .....	2 Report
PLAT213_ALERT_2_B Atom O2 has ADP max/min Ratio .....	4.4 oblate
PLAT213_ALERT_2_B Atom C6 has ADP max/min Ratio .....	5.0 oblate
PLAT213_ALERT_2_B Atom C8 has ADP max/min Ratio .....	4.2 oblate
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds .....	0.03294 Ang.

### Alert level C

DIFMN02\_ALERT\_2\_C The minimum difference density is < -0.1\*ZMAX\*0.75  
 \_refine\_diff\_density\_min given = -3.325  
 Test value = -3.150

DIFMN03\_ALERT\_1\_C The minimum difference density is < -0.1\*ZMAX\*0.75  
 The relevant atom site should be identified.

DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75  
 The relevant atom site should be identified.

GOODF01\_ALERT\_2\_C The least squares goodness of fit parameter lies  
 outside the range 0.80 <> 2.00  
 Goodness of fit given = 2.389

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT087_ALERT_2_C Unsatisfactory S value (Too High) .....	2.39 Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....	3.29 Report
PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density	-3.33 eA-3
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .....	7 Check
PLAT213_ALERT_2_C Atom O3 has ADP max/min Ratio .....	3.3 prolat
PLAT213_ALERT_2_C Atom C5 has ADP max/min Ratio .....	3.1 prolat
PLAT234_ALERT_4_C Large Hirshfeld Difference Mo1 --C2 .	0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Mn2 --C5 .	0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O2 --C2 .	0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C17 --C22 .	0.19 Ang.
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....	2.5 Note
PLAT353_ALERT_3_C Long N-H (N0.87,N1.01A) N1 - H4 .	1.01 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor N1 --H3 .	Please Check
PLAT751_ALERT_4_C Bond Calc 1.56000, Rep 1.5625(14) .....	Senseless s.u.
MO1 -H1 1.555 1.555 .....	# 10 Check
PLAT751_ALERT_4_C Bond Calc 1.82000, Rep 1.824(3) .....	Senseless s.u.
MN2 -H1 1.555 1.555 .....	# 16 Check
PLAT751_ALERT_4_C Bond Calc 0.99000, Rep 0.995(14) .....	Senseless s.u.
N1 -H2 1.555 1.555 .....	# 19 Check
PLAT751_ALERT_4_C Bond Calc 1.00000, Rep 0.997(13) .....	Senseless s.u.
N1 -H3 1.555 1.555 .....	# 20 Check
PLAT752_ALERT_4_C Angle Calc 137.00, Rep 137.2(7) .....	Senseless s.u.
C1 -MO1 -H1 1.555 1.555 1.555	# 37 Check
PLAT752_ALERT_4_C Angle Calc 82.00, Rep 82.4(6) .....	Senseless s.u.
C2 -MO1 -H1 1.555 1.555 1.555	# 38 Check
PLAT752_ALERT_4_C Angle Calc 129.00, Rep 129.0(6) .....	Senseless s.u.
C8 -MO1 -H1 1.555 1.555 1.555	# 39 Check
PLAT752_ALERT_4_C Angle Calc 130.00, Rep 129.9(7) .....	Senseless s.u.

C9	-MO1	-H1	1.555	1.555	1.555	# 40 Check
PLAT752_ALERT_4_C	Angle	Calc	96.00, Rep	95.7(6)	.....	Senseless s.u.
C10	-MO1	-H1	1.555	1.555	1.555	# 41 Check
PLAT752_ALERT_4_C	Angle	Calc	93.00, Rep	93.5(6)	.....	Senseless s.u.
C7	-MO1	-H1	1.555	1.555	1.555	# 42 Check
PLAT752_ALERT_4_C	Angle	Calc	76.00, Rep	75.8(5)	.....	Senseless s.u.
C6	-MO1	-H1	1.555	1.555	1.555	# 43 Check
PLAT752_ALERT_4_C	Angle	Calc	73.00, Rep	73.12(12)	.....	Senseless s.u.
P1	-MO1	-H1	1.555	1.555	1.555	# 44 Check
PLAT752_ALERT_4_C	Angle	Calc	26.00, Rep	26.36(6)	.....	Senseless s.u.
MN2	-MO1	-H1	1.555	1.555	1.555	# 45 Check
PLAT752_ALERT_4_C	Angle	Calc	172.00, Rep	171.8(7)	.....	Senseless s.u.
C3	-MN2	-H1	1.555	1.555	1.555	# 61 Check
PLAT752_ALERT_4_C	Angle	Calc	89.00, Rep	88.9(6)	.....	Senseless s.u.
C5	-MN2	-H1	1.555	1.555	1.555	# 62 Check
PLAT752_ALERT_4_C	Angle	Calc	92.00, Rep	91.6(9)	.....	Senseless s.u.
C4	-MN2	-H1	1.555	1.555	1.555	# 63 Check
PLAT752_ALERT_4_C	Angle	Calc	91.00, Rep	91.2(4)	.....	Senseless s.u.
N1	-MN2	-H1	1.555	1.555	1.555	# 64 Check
PLAT752_ALERT_4_C	Angle	Calc	74.00, Rep	73.88(14)	.....	Senseless s.u.
P1	-MN2	-H1	1.555	1.555	1.555	# 65 Check
PLAT752_ALERT_4_C	Angle	Calc	22.00, Rep	22.36(5)	.....	Senseless s.u.
MO1	-MN2	-H1	1.555	1.555	1.555	# 66 Check
PLAT752_ALERT_4_C	Angle	Calc	136.00, Rep	136.0(12)	.....	Senseless s.u.
MN2	-N1	-H2	1.555	1.555	1.555	# 73 Check
PLAT752_ALERT_4_C	Angle	Calc	113.00, Rep	113.0(10)	.....	Senseless s.u.
MN2	-N1	-H3	1.555	1.555	1.555	# 74 Check
PLAT752_ALERT_4_C	Angle	Calc	97.00, Rep	97.5(12)	.....	Senseless s.u.
H2	-N1	-H3	1.555	1.555	1.555	# 75 Check
PLAT752_ALERT_4_C	Angle	Calc	106.00, Rep	106(3)	.....	Senseless s.u.
H2	-N1	-H4	1.555	1.555	1.555	# 77 Check
PLAT752_ALERT_4_C	Angle	Calc	106.00, Rep	106(3)	.....	Senseless s.u.
H3	-N1	-H4	1.555	1.555	1.555	# 78 Check



## Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	6 Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	2 Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.20 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3 Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	2 Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2 Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C30	Constrained at 0.7 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C31	Constrained at 0.7 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C32	Constrained at 0.7 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C33	Constrained at 0.7 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C34	Constrained at 0.7 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C35	Constrained at 0.7 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C36	Constrained at 0.7 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H30A	Constrained at 0.7 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H30B	Constrained at 0.7 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H30C	Constrained at 0.7 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H32	Constrained at 0.7 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H33	Constrained at 0.7 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H34	Constrained at 0.7 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H35	Constrained at 0.7 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H36	Constrained at 0.7 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C30B	Constrained at 0.3 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C31B	Constrained at 0.3 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C32B	Constrained at 0.3 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of C33B	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C34B	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C35B	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C36B	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H30D	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H30E	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H30F	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H32B	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H33B	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H34B	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H35B	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H36B	Constrained at	0.3	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )		100%	Note
PLAT303_ALERT_2_G	Full Occupancy Atom H1 with # Connections		2.00	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 2		10.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 3		4.50	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety .....		C30	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn2 (I) .		0.92	Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters		1	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		24	Note

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 21 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 5 ALERT type 3 Indicator that the structure quality may be low  
 67 ALERT type 4 Improvement, methodology, query or suggestion  
 2 ALERT type 5 Informative message, check

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## Datablock: compound3a

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Bond precision: C-C = 0.0042 A                      Wavelength=1.54184

Cell:                      a=10.9412(6)                      b=11.1757(6)                      c=11.9618(6)  
                                  alpha=84.979(4)                      beta=78.905(5)                      gamma=84.550(4)

Temperature: 156 K

	Calculated	Reported
Volume	1425.22(13)	1425.22(13)
Space group	P -1	P -1
Hall group	: -P 1	-P 1
Moiety formula	C31 H25 Mn Mo N O5 P	C31 H25 Mn Mo N O5 P
Sum formula	C31 H25 Mn Mo N O5 P	C31 H25 Mn Mo N O5 P
Mr	673.37	673.37
Dx,g cm-3	1.569	1.569
Z	2	2
Mu (mm-1)	8.080	8.080
F000	680.0	680.0
F000'	681.06	
h,k,lmax	13,13,14	13,13,14
Nref	5376	5243
Tmin,Tmax	0.296,0.524	0.739,1.000
Tmin'	0.136	

Correction method= # Reported T Limits: Tmin=0.739 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.975                      Theta(max)= 69.691

R(reflections)= 0.0276( 4743)              wR2(reflections)= 0.0752( 5243)

S = 1.058                                      Npar= 367

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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 G

PLAT230_ALERT_2_G	Hirshfeld Test Diff for	O1	--C1	.	7.3 s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	O2	--C2	.	7.4 s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	O3	--C3	.	5.2 s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	O4	--C4	.	5.4 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Mo1	--C1	.	10.9 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Mo1	--C2	.	9.7 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Mn1	--C3	.	9.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Mn1	--C4	.	9.5 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Mn1	--C5	.	7.8 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Mn1	--C6	.	7.6 s.u.
PLAT303_ALERT_2_G	Full Occupancy Atom H1		with # Connections		2.00 Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn1		(I)	.	0.96 Info

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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  
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
12 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

11 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 ALERT type 3 Indicator that the structure quality may be low  
0 ALERT type 4 Improvement, methodology, query or suggestion  
1 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* 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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**PLATON version of 26/09/2018; check.def file version of 13/09/2018**



