

Structure factors have been supplied for datablock(s) shelx

No syntax errors found. CIF dictionary Interpreting this report

Bond precision:	C-C = 0.0032 A	Wavelength=1.54178	
Cell:	a=19.2401 (10)	b=12.1579 (7)	c=10.1312 (6)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	2369.9 (2)	2369.9 (2)	
Space group	P b c n	P b c n	
Hall group	-P 2n 2ab	-P 2n 2ab	
Moiety formula	C24 H28 Mn N4 O5	?	
Sum formula	C24 H28 Mn N4 O5	C24 H28 Mn N4 O5	
Mr	507.44	507.44	
Dx, g cm-3	1.422	1.422	
Z	4	4	
Mu (mm-1)	4.893	4.893	
F000	1060.0	1060.0	
F000'	1060.97		
h, k, lmax	23, 14, 12	23, 14, 12	
Nref	2171	2136	
Tmin, Tmax	0.256, 0.294	0.253, 0.753	
Tmin'	0.088		

Data completeness= 0.984                      Theta (max)= 68.225

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R(reflections)= 0.0414( 2037)      wR2(reflections)=
S = 1.086                        0.1133( 2136)
Npar= 161
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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.

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### Alert level C

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min)	Range	3.3	Ratio
PLAT250_ALERT_2_C	Large U3/U1	Ratio for <U(i,j)>	Tensor(Resd 1)			2.7	Note
PLAT911_ALERT_3_C	Missing FCF	Refl Between Thmin & STh/L=	0.600			32	Report
	0 4 0,	2 2 0,	3 5 0,	8 12 0,	10 0 0,	15 9 0,	
	16 8 0,	17 9 0,	19 5 0,	0 2 1,	1 2 1,	4 1 1,	
	5 1 1,	6 1 1,	4 6 2,	8 12 2,	12 0 2,	20 0 2,	
	6 2 3,	13 11 3,	16 8 3,	0 0 4,	11 9 4,	20 0 4,	
	13 7 7,	15 7 7,	12 2 9,	8 0 10,	10 0 10,	0 2 11,	
	8 2 11,	0 0 12,					

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### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	3	Report
	H1A H1B H2		
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Mn1 --O2 .	5.4	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of H1A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1B Constrained at	0.5	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	10.30	Deg.
	H1A -O1 -H1B 1_555 1_555 3_655 ..... #	17	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	10.30	Deg.
	H1B -O1 -H1A 1_555 1_555 3_655 ..... #	19	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	1	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3	Note
	1 1 0, 2 0 0, 1 1 1,		
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	3	Note
	2 0 0, 0 2 1, 5 1 1,		
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	8	Note
	0 2 1, 5 1 1, 4 1 1, 1 1 0, 0 0 4, 20 0 2,		
	1 2 1, 12 0 2,		
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....	3.61	Note
	Predicted wR2: Based on SigI**2 3.14 or SHELX Weight 10.84		
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	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  
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
17 **ALERT level G** = General information/check it is not something unexpected

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
7 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  
6 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

