

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision: C-C = 0.0068 Å Wavelength=1.54178

Cell: a=10.6563(18) b=10.9066(19) c=12.790(2)
 alpha=89.159(9) beta=66.391(7) gamma=86.483(8)

Temperature: 100 K

	Calculated	Reported
Volume	1359.4(4)	1359.4(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 H16 Cl2 Mn N4, C7 H5 Cl O2	?
Sum formula	C31 H21 Cl3 Mn N4 O2	C31 H21 Cl3 Mn N4 O2
Mr	642.81	642.81
Dx, g cm ⁻³	1.570	1.570
Z	2	2
Mu (mm ⁻¹)	6.977	6.977
F000	654.0	654.0
F000'	656.67	
h,k,lmax	12,13,15	12,13,15
Nref	5041	4832
Tmin,Tmax	0.144,0.175	0.366,0.753
Tmin'	0.047	

Correction method= # Reported T Limits: Tmin=0.366 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.959 Theta(max)= 68.914

R(reflections)= 0.0773(4543)

wR2(reflections)=
0.2233(4832)

S = 1.060

Npar= 371

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

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full value Low . 0.967 Why?
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 3.0 Note
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00684 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 163 Report

1	1	0,	-1	2	0,	1	2	0,	2	2	0,	3	2	0,	-1	3	0,
0	3	0,	11	3	0,	-1	4	0,	0	4	0,	-2	5	0,	0	5	0,
10	6	0,	-1	-6	1,	0	-6	1,	-1	-5	1,	0	-5	1,	-4	-4	1,
-3	-4	1,	0	-4	1,	1	-4	1,	4	-4	1,	-11	-3	1,	-9	-3	1,
-2	-3	1,	2	-3	1,	-3	-2	1,	-1	-2	1,	0	-2	1,	1	-2	1,
0	-1	1,	-6	2	1,	1	2	1,	2	2	1,	11	2	1,	2	3	1,
-3	5	1,	-2	5	1,	-2	6	1,	0	6	1,	1	6	1,	9	9	1,
4	-12	2,	3	-5	2,	4	-5	2,	0	-4	2,	1	-4	2,	2	-4	2,
4	-4	2,	-2	-3	2,	1	-3	2,	2	-3	2,	3	-3	2,	-1	-2	2,
-4	-1	2,	1	-1	2,	1	0	2,	3	0	2,	-1	1	2,	1	2	2,
1	3	2,	11	3	2,	-1	4	2,	3	4	2,	-2	5	2,	-1	5	2,
0	5	2,	3	5	2,	4	5	2,	-1	6	2,	0	6	2,	10	8	2,
7	10	2,	3	-12	3,	4	-12	3,	3	-5	3,	-3	-4	3,	0	-4	3,
1	-4	3,	2	-4	3,	-2	-3	3,	-3	-2	3,	1	-2	3,	2	-2	3,
1	-1	3,	1	2	3,	2	3	3,	-2	4	3,	-1	4	3,	3	4	3,
11	7	3,	3	-12	4,	4	-12	4,	-2	-4	4,	0	-4	4,	4	-4	4,

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1 Report
H1
PLAT794_ALERT_5_G Tentative Bond Valency for Mn1 (II) . 2.04 Info
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). 1 Note
0 0 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 44 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 3 Note
0 3 0, 0 4 0, 3 0 2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.3 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 4.49 Note
Predicted wR2: Based on SigI**2 4.97 or SHELX Weight 21.92
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **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
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
2 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* 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.

