

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: 1

Bond precision: C-C = 0.0155 A Wavelength=0.71073

Cell: a=10.156(9) b=12.088(11) c=12.765(11)
 alpha=112.668(15) beta=102.560(17) gamma=96.464(17)
Temperature: 293 K

	Calculated	Reported
Volume	1378(2)	1377(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C21 H14 Mn N3 O7 [+ solvent]	C21 H14 Mn N3 O7
Sum formula	C21 H14 Mn N3 O7 [+ solvent]	C21 H14 Mn N3 O7
Mr	475.29	475.29
Dx, g cm ⁻³	1.145	1.146
Z	2	2
Mu (mm ⁻¹)	0.516	0.516
F000	484.0	484.0
F000'	484.91	
h, k, lmax	13, 15, 16	13, 15, 16
Nref	6522	5991
Tmin, Tmax	0.930, 0.950	0.526, 0.746
Tmin'	0.930	

Correction method= # Reported T Limits: Tmin=0.526 Tmax=0.746

AbsCorr = MULTI-SCAN

Data completeness= 0.919

Theta(max)= 27.795

R(reflections)= 0.1353(2926)

wR2(reflections)=
0.3940(5991)

S = 1.119

Npar= 293

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

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) 0.39 Report

Author Response: Due to the poor signal-to-noise ratio of the crystal.

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.0155 Ang.

Author Response: Du to the poor quality of the crystal.



Alert level C

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 49% Check
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.960 Why?
PLAT082_ALERT_2_C High R1 Value 0.14 Report
PLAT213_ALERT_2_C Atom O2 has ADP max/min Ratio 3.4 oblate
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.5 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 10.0 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C2 --C3 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C11 --C12 . 0.19 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 06 Check
PLAT245_ALERT_2_C U(iso) H3 Smaller than U(eq) O3 by 0.045 Ang**2
PLAT420_ALERT_2_C D-H Bond Without Acceptor N2 --H2 . Please Check



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 3 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
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C18 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mn1 (II) . 1.86 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 15 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 1.2 Low

0 **ALERT level A** = Most likely a serious problem - resolve or explain

2 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
14 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
3 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* 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.

PLATON version of 13/07/2021; check.def file version of 13/07/2021

Datablock 1 - ellipsoid plot

