Datablock: 2

Bond precision: C-C = 0.0040 A   Wavelength=0.71073

Cell: a=9.6427(5)   b=10.8396(5)   c=10.8617(8)
             alpha=106.971(5)beta=103.497(5) gamma=112.469(5)

Temperature
:   293 K

	Calculated	Reported
Volume	923.85(12)	923.85(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C20 H32 Mn2 N20 O2 S2, 2(C H4 O)	?
Sum formula	C22 H40 Mn2 N20 O4 S2	C22 H40 Mn2 N20 O4 S2
Mr	822.74	822.74
Dx,g cm-3	1.479	1.479
Z	1	1
Mu (mm-1)	0.856	0.856
F000	426.0	426.0
F000'	427.02	
h,k,lmax	12,14,14	12,14,14
Nref	4233	4144
Tmin,Tmax	0.717,0.843	0.780,1.000
Tmin'	0.703	

Correction method= # Reported T Limits: Tmin=0.780
Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 0.979   Theta(max)= 27.484

R(reflections)= 0.0371(3319)   wR2(reflections)= 0.0982(4144)

S = 1.072   Npar= 232

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

PLAT220_ALERT_2_C	NonSolvent Resd 1 N Ueq(max)/Ueq(min) Range	3.2	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	N5	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	N8	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Mn1	Check

And 3 other PLAT242 Alerts

PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	N4	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	N6	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	N9	Check

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🔘 Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	2	Units
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.005	Degree
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn1 (II) .	2.12	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	87	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.4	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	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
   7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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  11 ALERT level G = General information/check it is not something unexpected

  5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  8 ALERT type 2 Indicator that the structure model may be wrong or deficient
  2 ALERT type 3 Indicator that the structure quality may be low
  1 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* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.
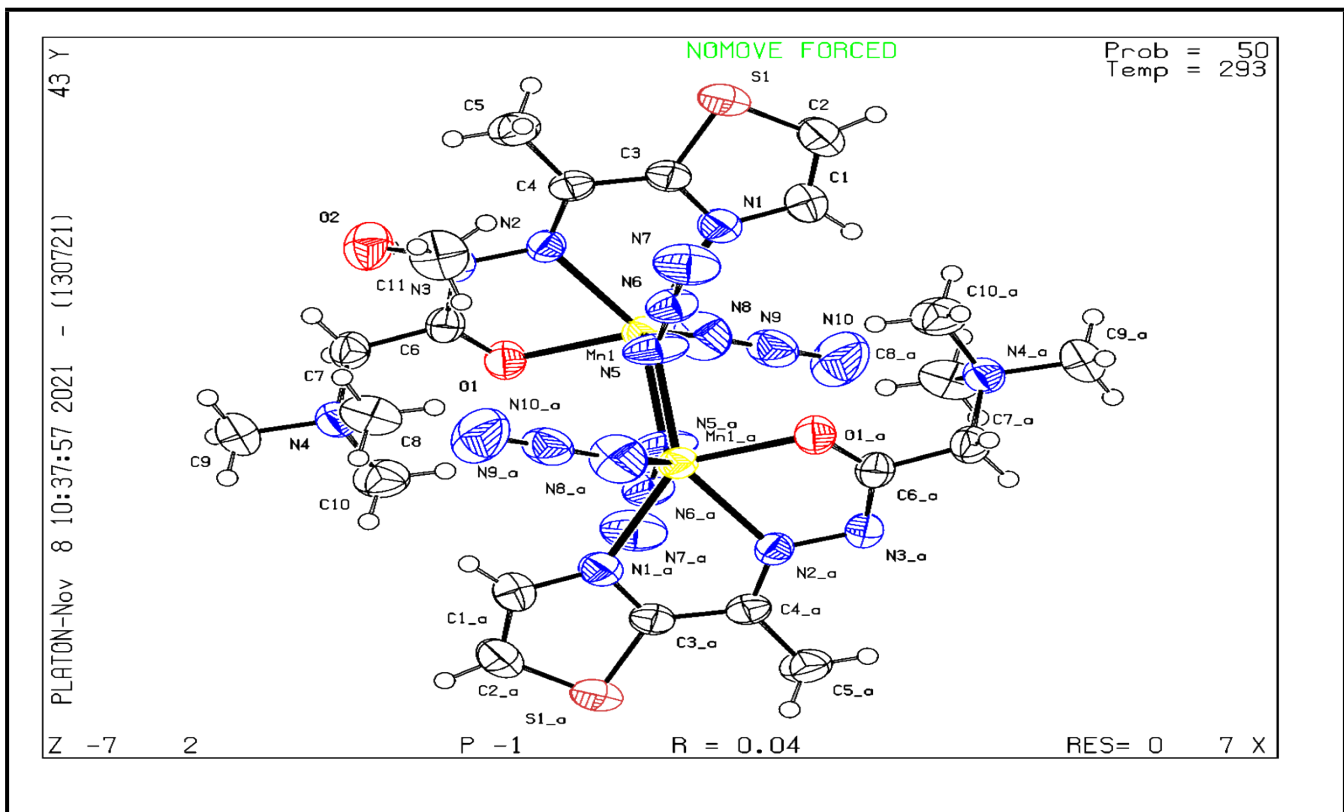
Publication of your CIF in other journals

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 2 - ellipsoid plot