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 = 0.0065 A          Wavelength=0.71073

Cell:              a=20.651(3)      b=20.651(3)      c=13.641(3)
                   alpha=90         beta=90          gamma=90
Temperature:       293 K
```

	Calculated	Reported
Volume	5817(2)	5818(2)
Space group	P 42/n	P 42/n
Hall group	-P 4bc	-P 4bc
Moiety formula	C58 H36 Fe2 Mn N12 O14	?
Sum formula	C58 H36 Fe2 Mn N12 O14	C58 H44 Fe2 Mn N12 O14
Mr	1291.63	1299.69
Dx,g cm-3	1.475	1.484
Z	4	4
Mu (mm-1)	0.783	0.783
F000	2628.0	2660.0
F000’	2633.20	
h,k,lmax	26,26,17	26,26,17
Nref	6650	6637
Tmin,Tmax	0.855,0.889	0.347,1.000
Tmin’	0.855	

```
Correction method= # Reported T Limits: Tmin=0.347 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.998          Theta(max)= 27.450

R(reflections)= 0.0579( 3771)     wR2(reflections)= 0.1972( 6637)

S = 1.090                 Npar= 412
```

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

```
PLAT601_ALERT_2_B Unit Cell Contains Solvent Accessible VOIDS of .        108 Ang**3
```

Alert level C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       8.06 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT234_ALERT_4_C Large Hirshfeld Difference O7B      --C29B     .       0.18 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Mn1 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00654 Ang.
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Alert level G

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FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C58 H44 Fe2 Mn1 N12 O14
           Atom count from the _atom_site data:  C58 H36 Fe2 Mn1 N12 O14
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C58 H44 Fe2 Mn N12 O14
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        232.00    232.00    0.00
          H        176.00    144.00   32.00
          Fe         8.00      8.00    0.00
          Mn         4.00      4.00    0.00
          N         48.00     48.00    0.00
          O         56.00     56.00    0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe1      --N3       .        6.4 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         5% Note
PLAT315_ALERT_2_G Singly Bonded Carbon Detected (H-atoms Missing).       C29B Check
PLAT315_ALERT_2_G Singly Bonded Carbon Detected (H-atoms Missing).       C29A Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
```

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

   8 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
   1 ALERT type 5 Informative message, check
```

Datablock: 2

Bond precision: C-C = 0.0063 A Wavelength=0.71073

Cell:	a=9.2247(6)	b=13.2300(7)	c=14.2577(8)
	alpha=82.3377(15)	beta=79.666(2)	gamma=85.466(2)
Temperature:	293 K		

	Calculated	Reported
Volume	1693.82(17)	1693.83(17)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C62 H50 Mn3 N14 O14, 2(C3 H7 N O)	?
Sum formula	C68 H64 Mn3 N16 O16	C68 H64 Mn3 N16 O16
Mr	1526.17	1526.17
Dx,g cm-3	1.496	1.496
Z	1	1
Mu (mm-1)	0.633	0.633
F000	787.0	787.0
F000’	788.33	
h,k,lmax	11,17,18	11,17,18
Nref	7754	7655
Tmin,Tmax	0.872,0.939	0.057,1.000
Tmin’	0.710	

Correction method= # Reported T Limits: Tmin=0.057 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.987 Theta(max)= 27.483

R(reflections)= 0.0485(4597) wR2(reflections)= 0.1631(7655)

S = 1.153 Npar= 467

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

PLAT230_ALERT_2_C Hirshfeld Test Diff for O6 --N6 . 5.5 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C12 --C13 . 5.5 s.u.
PLAT241_ALERT_2_C High ’MainMol’ Ueq as Compared to Neighbors of O2 Check
PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of Mn2 Check
PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of N7 Check
PLAT244_ALERT_4_C Low ’Solvent’ Ueq as Compared to Neighbors of N8 Check
PLAT244_ALERT_4_C Low ’Solvent’ Ueq as Compared to Neighbors of C32 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O8 0.106 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00629 Ang.

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check

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PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C30 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C33 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C34 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Mn1       (I)       .       1.02 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mn2       (II)      .       2.20 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         20 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.2 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please 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

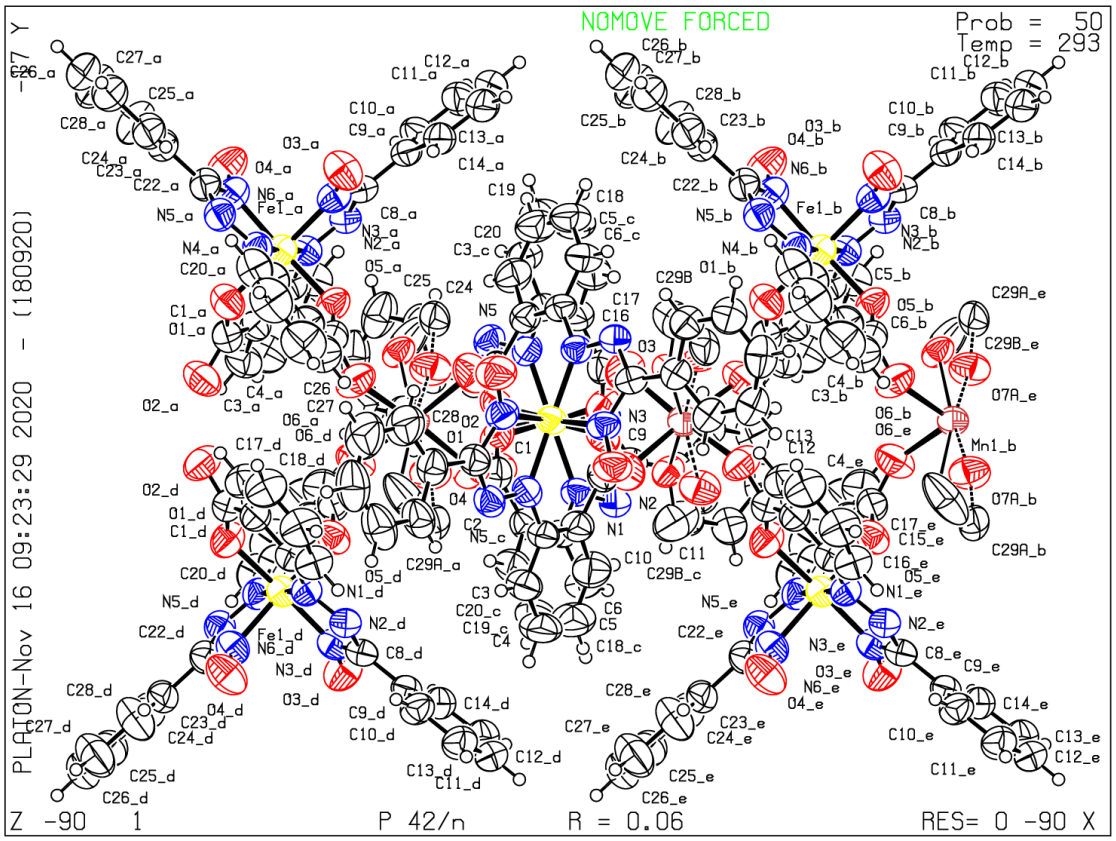
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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.

PLATON version of 18/09/2020; check.def file version of 20/08/2020

Datablock 1 - ellipsoid plot



Datablock 2 - ellipsoid plot