

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) test

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: test

Bond precision:	C-C = 0.0101 Å	Wavelength=0.71073
Cell:	a=14.3852(11) b=15.3085(11) c=21.6557(17)	
	alpha=90 beta=105.645(1) gamma=90	
Temperature:	293 K	
	Calculated	Reported
Volume	4592.2(6)	4592.2(6)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
	C41 H33 Fe Mn N9 O3, C	
Moiety formula	H1.50 N0.50, C0.50 H2 O0.50, C H4 O, H0.	?
Sum formula	C43.50 H41 Fe Mn N9.50 O4.75	C43.50 H41 Fe Mn N9.50 O4.75
Mr	883.65	883.65
Dx, g cm ⁻³	1.278	1.278
Z	4	4
Mu (mm ⁻¹)	0.643	0.643
F000	1830.0	1830.0
F000'	1833.32	
h,k,lmax	17,18,25	17,18,25
Nref	8096	8062
Tmin,Tmax	0.837,0.891	0.825,0.894
Tmin'	0.819	

Correction method= # Reported T Limits: Tmin=0.825 Tmax=0.894
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 25.009

R(reflections)= 0.0777(6079) wR2(reflections)= 0.2482(8062)

S = 1.041 Npar= 577

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

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.35	Report
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	2.12	eA-3
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference N7 --C11 .	0.17	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of N7		Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C29		Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C34		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C9		Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of C11		Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including N10	0.106	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including O6	0.121	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including O5	0.134	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01006	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.595	32	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	2	Check
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers	1	Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.82A From Fe1	2.07	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.94A From O5	1.23	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.61A From O5	1.04	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.67A From O5	1.04	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.06A From O5	0.89	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.05A From N7	0.51	eA-3

● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	8	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4	Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.14	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	9.83	Why ?
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	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
PLAT300_ALERT_4_G	Atom Site Occupancy of N10 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C45 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C46 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H47A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H47B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H47C Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O4 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C43 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43C Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O5 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5B Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5C Constrained at	0.25	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note

PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C4 -C9	0.17	Ang.
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (III)	3.31	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn1 (I)	0.82	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	21	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary		Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	49%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	2	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	30	Note
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
23 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
38 **ALERT level G** = General information/check it is not something unexpected

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

