

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 = 0.0049 A	Wavelength=0.71073	
Cell:	a=16.8839(6)	b=25.7793(6)	c=62.8204(17)
	alpha=90	beta=90	gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	27342.9(14)	27342.9(14)	
Space group	F d d d	F d d d	
Hall group	-F 2uv 2vw	-F 2uv 2vw	
Moiety formula	C48 H72 B2 Fe2 Mn N22 [+ solvent]	C48 H72 B2 Fe2 Mn N22	
Sum formula	C48 H72 B2 Fe2 Mn N22 [+ solvent]	C48 H72 B2 Fe2 Mn N22	
Mr	1145.54	1145.53	
Dx, g cm ⁻³	1.113	1.113	
Z	16	16	
Mu (mm ⁻¹)	0.646	0.646	
F000	9616.0	9616.0	
F000'	9634.23		
h,k,lmax	20,30,74	20,30,74	
Nref	6043	6041	
Tmin,Tmax	0.824,0.824	0.632,0.746	
Tmin'	0.824		
Correction method= # Reported T Limits: Tmin=0.632 Tmax=0.746			
AbsCorr = MULTI-SCAN			
Data completeness=	1.000	Theta(max)=	24.997
R(reflections)=	0.0433(4400)	wR2(reflections)=	0.1303(6041)
S =	1.103	Npar=	351

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	Non-Solvent	Resd 1	C	Ueq(max)/Ueq(min) Range	3.3	Ratio
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C21	Check	
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C22	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Mn1	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	N10	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	N11	Check	
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond	C21 - C22	1.34	Ang.	
PLAT410_ALERT_2_C	Short	Intra H...H Contact	H21A ..H22B	1.97	Ang.	
PLAT410_ALERT_2_C	Short	Intra H...H Contact	H21B ..H22A	1.98	Ang.	

● **Alert level G**

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	2	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	17.96	Why ?
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Fel --C16	7.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Fel --C17	6.2	s.u.
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C5	Check
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	12	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	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
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
13 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

PLATON version of 30/01/2018; check.def file version of 30/01/2018

