

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 287c

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: 287c

Bond precision: C-C = 0.0362 A Wavelength=0.71073

Cell: a=19.8840(19) b=7.6471(6) c=23.415(2)
 alpha=90 beta=98.946(9) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	3517.1(5)	3517.1(6)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C15 H21 Mn O6	C15 H21 Mn O6
Sum formula	C15 H21 Mn O6	C15 H21 Mn O6
Mr	352.26	352.26
Dx,g cm-3	1.331	1.330
Z	8	8
Mu (mm-1)	0.774	0.773
F000	1472.0	1472.0
F000'	1475.42	
h,k,lmax	23,9,27	23,9,27
Nref	12545[6787]	12441
Tmin,Tmax	0.895,0.938	0.475,1.000
Tmin'	0.735	

Correction method= # Reported T Limits: Tmin=0.475 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.83/0.99 Theta(max)= 25.122

R(reflections)= 0.0961(3926) wR2(reflections)= 0.2820(12441)

S = 0.893 Npar= 817

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 A

EXPT005_ALERT_1_A _exptl_crystal_description is missing
Crystal habit description.
The following tests will not be performed.
CRYSR_01

RINTA01_ALERT_3_A The value of Rint is greater than 0.25
Rint given 0.298

SHFSU01_ALERT_2_A The absolute value of parameter shift to su ratio > 0.20
Absolute value of the parameter shift to su ratio given 0.439
Additional refinement cycles may be required.

PLAT020_ALERT_3_A The Value of Rint is Greater Than 0.12 0.298 Report
PLAT080_ALERT_2_A Maximum Shift/Error 0.44 Why ?
PLAT213_ALERT_2_A Atom C27 has ADP max/min Ratio 5.6 prolat
PLAT213_ALERT_2_A Atom C57 has ADP max/min Ratio 13.0 prolat
PLAT213_ALERT_2_A Atom C59 has ADP max/min Ratio 5.5 prolat
PLAT234_ALERT_4_A Large Hirshfeld Difference C22 --C23 . 0.32 Ang.
PLAT234_ALERT_4_A Large Hirshfeld Difference C56 --C57 . 0.32 Ang.
PLAT234_ALERT_4_A Large Hirshfeld Difference C58 --C59 . 0.33 Ang.
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value Please Do !

Alert level B

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low .. 32% Check
PLAT234_ALERT_4_B Large Hirshfeld Difference C6 --C7 . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C9 --C10 . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C12 --C13 . 0.30 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C8 --C19 . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C011 --C27 . 0.28 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C17 --C18 . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C27 --C28 . 0.28 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C29 --C30 . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C015 --C37 . 0.28 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C52 --C53 . 0.28 Ang.
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.03625 Ang.
PLAT987_ALERT_1_B The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

Alert level C

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.560
From the CIF: _refine_ls_abs_structure_Flack_su 0.090

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.28 Report
PLAT112_ALERT_2_C ADDSYM Detects New (Pseudo) Symm. Elem B 80 %Fit
PLAT112_ALERT_2_C ADDSYM Detects New (Pseudo) Symm. Elem B 80 %Fit
PLAT213_ALERT_2_C Atom C2 has ADP max/min Ratio 3.8 prolat
PLAT213_ALERT_2_C Atom C12 has ADP max/min Ratio 3.2 prolat
PLAT213_ALERT_2_C Atom C32 has ADP max/min Ratio 4.0 oblate
PLAT213_ALERT_2_C Atom C54 has ADP max/min Ratio 3.8 prolat
PLAT234_ALERT_4_C Large Hirshfeld Difference C04 --C9 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C8 --C9 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C11 --C12 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C012 --C29 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C013 --C32 . 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C014 --C34 . 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Mn4 --O20 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C59 --C60 . 0.22 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 06 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 011 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 012 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C23 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 019 Check

PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C58	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C4	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C7	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C12	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C14	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C22	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C24	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C42	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C47	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C52	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C57	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C59	Check
PLAT413_ALERT_2_C	Short Inter	XH3 .. XHn	Hi ..Hw .	2.10	Ang.
			x,-1+y,z =	1_545	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		9.475	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		2.024	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		3.298	Check
PLAT907_ALERT_2_C	Flack x > 0.5, Structure Needs to be Inverted?	.		0.56	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.597		4	Report

● Alert level G

PLAT012_ALERT_1_G	No	_shelx_res_checksum	Found in CIF	Please Check
PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero	.		0.560	Note
PLAT115_ALERT_5_G	ADDSYM Detects Noncrystallographic Inversion	...		80%	Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)		293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)		293	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		26	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn1	(I) .		0.95	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn2	(I) .		0.94	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn3	(I) .		0.92	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn4	(I) .		0.93	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).			4	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File	...		6	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			0	Info

-
- 12 **ALERT level A** = Most likely a serious problem - resolve or explain
13 **ALERT level B** = A potentially serious problem, consider carefully
39 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected
- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
32 ALERT type 2 Indicator that the structure model may be wrong or deficient
10 ALERT type 3 Indicator that the structure quality may be low
24 ALERT type 4 Improvement, methodology, query or suggestion
5 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 05/12/2020; check.def file version of 05/12/2020

