

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) c_sc_068_final

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: c_sc_068_final

Bond precision:	C-C = 0.0167 Å	Wavelength=1.54178
Cell:	a=11.820(1)	b=12.7584(11) c=13.3067(13)
	alpha=109.691(6)	beta=107.464(5) gamma=99.058(5)
Temperature:	100 K	
	Calculated	Reported
Volume	1726.0(3)	1726.0(3)
Space group	P 1	P 1
Hall group	P 1	P 1
	C17 H17 Cl Mn N5 O6, C17	
Moiety formula	H16 Cl Mn N5 O6, C17 H17 Mn C51 H50 Cl6 Mn3 N15 O31	
	N5 O3, 4(C	
Sum formula	C51 H50 Cl6 Mn3 N15 O31	C51 H50 Cl6 Mn3 N15 O31
Mr	1746.58	1746.58
Dx, g cm ⁻³	1.680	1.680
Z	1	1
Mu (mm ⁻¹)	7.409	7.409
F000	886.0	886.0
F000'	889.46	
h, k, lmax	14, 15, 16	14, 15, 16
Nref	14138[7069]	11220
Tmin, Tmax	0.317, 0.470	0.276, 0.519
Tmin'	0.154	

Correction method= # Reported T Limits: Tmin=0.276 Tmax=0.519

AbsCorr = MULTI-SCAN

Data completeness= 1.59/0.79

Theta(max)= 74.496

R(reflections) = 0.0693(9913)

wR2(reflections) =
0.1757(11220)

S = 1.034

Npar = 963

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

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds 0.01669 Ang.
PLAT354_ALERT_3_B Short O-H (X0.82,N0.98A) O3A - H31A . 0.58 Ang.

Alert level C

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.552
From the CIF: _refine_ls_abs_structure_Flack_su 0.010
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) 7.17 Note
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.1 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 061A Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.5 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.9 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 3.1 Note
PLAT354_ALERT_3_C Short O-H (X0.82,N0.98A) O2C - H21C . 0.65 Ang.
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O2B - H22B . 1.06 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C5B - C6B . 1.53 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C10C - C11C . 1.54 Ang.
PLAT415_ALERT_2_C Short Inter D-H..H-X H4A ..H22B . 2.03 Ang.

x,l+y,z = 1_565 Check
PLAT751_ALERT_4_C Bond Calc 0.89000, Rep 0.889(7) Senseless s.u.
O2A -H21A 1_555 1_555 # 18 Check
PLAT751_ALERT_4_C Bond Calc 0.58000, Rep 0.583(9) Senseless s.u.
O3A -H31A 1_555 1_555 # 19 Check
PLAT751_ALERT_4_C Bond Calc 0.81000, Rep 0.805(8) Senseless s.u.
O2B -H21B 1_555 1_555 # 65 Check
PLAT751_ALERT_4_C Bond Calc 1.06000, Rep 1.065(8) Senseless s.u.
O2B -H22B 1_555 1_555 # 66 Check
PLAT751_ALERT_4_C Bond Calc 0.65000, Rep 0.653(7) Senseless s.u.
O2C -H21C 1_555 1_555 # 112 Check
PLAT752_ALERT_4_C Angle Calc 113.00, Rep 112.9(7) Senseless s.u.
MN1A -O2A -H21A 1_555 1_555 1_555 # 29 Check
PLAT752_ALERT_4_C Angle Calc 129.00, Rep 128.6(12) Senseless s.u.
MN1A -O3A -H31A 1_555 1_555 1_555 # 30 Check
PLAT752_ALERT_4_C Angle Calc 129.00, Rep 128.7(7) Senseless s.u.
MN1B -O2B -H21B 1_555 1_555 1_555 # 114 Check
PLAT752_ALERT_4_C Angle Calc 129.00, Rep 129.4(6) Senseless s.u.
MN1B -O2B -H22B 1_555 1_555 1_555 # 115 Check
PLAT752_ALERT_4_C Angle Calc 98.00, Rep 98.4(8) Senseless s.u.
H21B -O2B -H22B 1_555 1_555 1_555 # 116 Check
PLAT752_ALERT_4_C Angle Calc 100.00, Rep 100.3(10) Senseless s.u.
MN1C -O2C -H21C 1_555 1_555 1_555 # 200 Check
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? . 0.55 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 101 Report

Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		5	Report
PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero .		0.552	Note
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		6.49	Why ?
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of			C12A Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of			C16A Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of			C11A Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of			C13A Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of			C14A Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of			C15A Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O11A ..C11A .		2.91	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O24A ..C1A .		2.98	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O41A ..C11B .		2.87	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O41A ..C10B .		2.93	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O64A ..C11A .		2.94	Ang.
		x,-1+y,1+z =	1_546	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		4	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn1A (II) .		2.25	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn1B (II) .		2.15	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn1C (II) .		2.25	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		63	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		4	Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged			Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by		4	Check

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 19 ALERT type 2 Indicator that the structure model may be wrong or deficient
 9 ALERT type 3 Indicator that the structure quality may be low
 19 ALERT type 4 Improvement, methodology, query or suggestion
 5 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
 _publ_contact_author_name and _publ_contact_author_address.
 PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
 _publ_contact_author_phone are all missing.

At least one of these should be present.
PUBL006_ALERT_1_A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.



Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.

7 **ALERT level A** = Data missing that is essential or data in wrong format
1 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
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;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_STRVA01_c_sc_068_final
;
PROBLEM: Flack test results are ambiguous.
RESPONSE: ...
;
_vrf_PLAT341_c_sc_068_final
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.01669 Ang.
RESPONSE: ...
;
_vrf_PLAT354_c_sc_068_final
;
PROBLEM: Short O-H (X0.82,N0.98A) O3A - H31A . 0.58 Ang.
RESPONSE: ...
;
_vrf_PLAT042_c_sc_068_final
;
PROBLEM: Calc. and Reported MoietyFormula Strings Differ Please Check
RESPONSE: ...
;
_vrf_PLAT090_c_sc_068_final
;
PROBLEM: Poor Data / Parameter Ratio (Zmax > 18) ..... 7.17 Note
RESPONSE: ...
;
_vrf_PLAT222_c_sc_068_final
;
PROBLEM: NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.1 Ratio
RESPONSE: ...
;
_vrf_PLAT241_c_sc_068_final

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;
PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of      061A Check
RESPONSE: ...
;
_vrf_PLAT250_c_sc_068_final
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....    2.5 Note
RESPONSE: ...
;
_vrf_PLAT355_c_sc_068_final
;
PROBLEM: Long O-H (X0.82,N0.98A) O2B - H22B . 1.06 Ang.
RESPONSE: ...
;
_vrf_PLAT369_c_sc_068_final
;
PROBLEM: Long C(sp2)-C(sp2) Bond C5B - C6B . 1.53 Ang.
RESPONSE: ...
;
_vrf_PLAT415_c_sc_068_final
;
PROBLEM: Short Inter D-H..H-X H4A ..H22B . 2.03 Ang.
RESPONSE: ...
;
_vrf_PLAT751_c_sc_068_final
;
PROBLEM: Bond Calc 0.89000, Rep 0.889(7) ..... Senseless s.u.
RESPONSE: ...
;
_vrf_PLAT752_c_sc_068_final
;
PROBLEM: Angle Calc 113.00, Rep 112.9(7) ..... Senseless s.u.
RESPONSE: ...
;
_vrf_PLAT907_c_sc_068_final
;
PROBLEM: Flack x > 0.5, Structure Needs to be Inverted? . 0.55 Check
RESPONSE: ...
;
_vrf_PLAT911_c_sc_068_final
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.600 101 Report
RESPONSE: ...
;
_vrf_PLAT915_c_sc_068_final
;
PROBLEM: No Flack x Check Done: Low Friedel Pair Coverage 61 %
RESPONSE: ...
;
# end Validation Reply Form

```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 06/07/2023; check.def file version of 30/06/2023

Datablock c_sc_068_final - ellipsoid plot

