

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAW160517

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: MAW160517

Bond precision: C-C = 0.0028 Å Wavelength=1.54184

Cell: a=7.0695(1) b=18.0623(2) c=12.1056(1)
 alpha=90 beta=97.105(1) gamma=90
Temperature: 183 K

	Calculated	Reported
Volume	1533.91(3)	1533.91(3)
Space group	P 21/m	P 21/m
Hall group	-P 2yb	-P 2yb
Moiety formula	C22 H21 N3 O2, 2(C2 H0.50 F3 O2), C2 H O2, Cl, 3(F)	?
Sum formula	C28 H23 Cl F9 N3 O8	C28 H23 Cl F9 N3 O8
Mr	735.94	735.94
Dx,g cm-3	1.593	1.593
Z	2	2
Mu (mm-1)	2.113	2.113
F000	748.0	748.0
F000'	751.93	
h,k,lmax	8,22,15	9,22,15
Nref	3412	3361
Tmin,Tmax	0.776,0.900	0.818,1.000
Tmin'	0.590	

Correction method= # Reported T Limits: Tmin=0.818 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.985 Theta(max)= 78.949

R(reflections)= 0.0480(3028) wR2(reflections)= 0.1428(3361)

S = 1.066 Npar= 317

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

PLAT430_ALERT_2_B Short Inter D...A Contact O32 .. O32 .. 2.77 Ang.

Alert level C

PLAT234_ALERT_4_C Large Hirshfeld Difference F25 -- C24 .. 0.17 Ang.
 PLAT234_ALERT_4_C Large Hirshfeld Difference F30 -- C24 .. 0.16 Ang.
 PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C21 Check
 PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.4 Note
 PLAT480_ALERT_4_C Long H...A H-Bond Reported H9 .. F39 .. 2.64 Ang.
 PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 2 Report

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 12 Note
 PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 10 Report
 PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 3 Report
 PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing 0.00010 Ang.
 PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
 PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 3 Report
 PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 2 Report
 PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C24 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of H14A is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of H14B is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of F25 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of F26 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of F27 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of F28 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of F29 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of F30 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of H23 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of O32 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of O33 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of C31 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of C34 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of H33 is Constrained at 0.5 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of F37 is Constrained at 0.7 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of F35 is Constrained at 0.35 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of F36 is Constrained at 0.35 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of F38 is Constrained at 0.15 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of F39 is Constrained at 0.15 Check
 PLAT300_ALERT_4_G Atom Site Occupancy of F40 is Constrained at 0.15 Check
 PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2).. 43 % 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
 PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6).. 100 % Note
 PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 7).. 100 % Note
 PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 8).. 100 % Note
 PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 9).. 100 % Note
 PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 10).. 100 % Note
 PLAT304_ALERT_4_G Non-Integer Number of Atoms (7.50) in Resd. # 2 Check
 PLAT304_ALERT_4_G Non-Integer Number of Atoms (2.50) in Resd. # 3 Check
 PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.50) in Resd. # 4 Check
 PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.35) in Resd. # 5 Check
 PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.35) in Resd. # 6 Check
 PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.35) in Resd. # 7 Check

PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.15)	in Resd. #	8	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.15)	in Resd. #	9	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.15)	in Resd. #	10	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond	C14 - C15	..	1.51	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F37 .. C34	..	1.40	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F37 .. C34	..	1.40	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F37 .. C31	..	2.32	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F37 .. C31	..	2.32	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O32 .. C31	..	1.63	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O32 .. C34	..	2.05	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O33 .. C31	..	0.94	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O33 .. C34	..	2.43	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F35 .. C34	..	1.35	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F35 .. C34	..	1.80	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F35 .. C31	..	2.14	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F35 .. C31	..	2.44	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F36 .. C34	..	1.10	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F36 .. C34	..	1.27	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F36 .. C31	..	2.34	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F36 .. C31	..	2.42	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F38 .. C34	..	1.04	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F38 .. C34	..	1.32	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F38 .. C31	..	2.35	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F38 .. C31	..	2.48	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F39 .. C34	..	1.28	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F39 .. C34	..	1.70	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F39 .. C31	..	2.05	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F39 .. C31	..	2.32	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F40 .. C34	..	1.37	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F40 .. C34	..	1.51	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F40 .. C31	..	2.24	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F40 .. C31	..	2.32	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C31 .. C31	..	0.44	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C31 .. C34	..	1.46	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C34 .. C34	..	0.46	Ang.
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)			1.20	Ratio
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms			!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints			75	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		50	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...			3	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			7	Note

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 38 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
 48 ALERT type 4 Improvement, methodology, query or suggestion
 2 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.

