

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_mo_ydg_lcf_oh_003_0m_a

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: mo_mo_ydg_lcf_oh_003_0m_a

Bond precision: C-C = 0.0061 A

Wavelength=0.71073

Cell: a=4.9126(7) b=9.9394(15) c=10.4255(15)
 alpha=103.125(5) beta=98.340(5) gamma=101.211(5)
Temperature: 303 K

	Calculated	Reported
Volume	476.67(12)	476.67(12)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C17 H19 F N6 O4, 2(H2 O)	C17 H19 F N6 O4, 2(H2 O)
Sum formula	C17 H23 F N6 O6	C17 H23 F N6 O6
Mr	426.41	426.41
Dx, g cm ⁻³	1.485	1.485
Z	1	1
Mu (mm ⁻¹)	0.120	0.120
F000	224.0	224.0
F000'	224.12	
h, k, lmax	6, 12, 13	6, 12, 13
Nref	4404[2202]	4237
Tmin, Tmax	0.980, 0.990	0.578, 0.746
Tmin'	0.951	

Correction method= # Reported T Limits: Tmin=0.578 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.92/0.96

Theta(max)= 27.528

R(reflections)= 0.0450(2959)

wR2(reflections)=
0.1013(4237)

S = 1.055

Npar= 280

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

STRVA01_ALERT_4_C Flack test results are meaningless.
 From the CIF: `_refine_ls_abs_structure_Flack` 0.200
 From the CIF: `_refine_ls_abs_structure_Flack_su` 0.600
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00607 Ang.
PLAT420_ALERT_2_C D-H Bond Without Acceptor N5 --H5A . Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor N6 --H6A . Please Check

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 11 Report
 H1 H3 H5A H5B H6A H6B H7 H00A H00B H00C H00D
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.600 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.005 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O2 . 109.8 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 6 Note
 O007 H00A H00B O00B H00C H00D
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
 H2 O
PLAT791_ALERT_4_G Model has Chirality at C7 (Sohncke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C8 (Sohncke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C10 (Sohncke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C11 (Sohncke SpGr) R Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 13 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 0.10 Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 1.707 Note
 Predicted wR2: Based on SigI**2 5.93 or SHELX Weight 9.60
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
9 ALERT type 4 Improvement, methodology, query or suggestion
3 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.

